新冠肺炎（COVID-19）中药天然产物计算筛选与文献证据集成分析

Natural Products for COVID-19 by Integrating Computational Screening and Literature Evidence

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[摘要]药物重定位（老药新用）策略在新发传染病中具有独特应用前景。我们前期提出了一种新的药物重定位系统——aCODE，可以基于疾病流行早期有限信息对潜在有效的天然产物进行预测。本文基于计算工具与文献证据，对可能在新冠病毒肺炎（COVID-19）防治中发挥作用的中药天然产物进行理论研究，发现：（1）文献调研共发现 56 种经过实验验证具有抗冠状病毒活性的天然产物成分，可靶向冠状病毒的结构蛋白和非结构蛋白；（2）将 aCODE 系统所预测的抗冠状病毒天然产物成分与文献证据对比，发现交集有大黄素、甘草酸、人参皂苷 R1、利血平和杨梅素等。大黄素可破坏冠状病毒 S 蛋白与宿主 ACE2 相互作用，阻止病毒入侵宿主细胞；同时具有抑制 3a 蛋白离子通道、阻止病毒释放的作用。甘草酸或其衍生物也是国内相关团队在新冠病毒肺炎治疗研究中重点关注的候选药物，已进入临床试验。(3) 针对中药预测结果中大量出现的芳香化合物，aCODE 系统增加芳香植物提取物数据源，计算发现氨基肉桂酸、肉桂醛、茴香烯、紫苏醇、芳樟醇、柠檬烯具有潜在的抗病毒效应。提示“芳香避秽”的细胞分子学机理值得进一步深入研究。

关键词：新冠肺炎；COVID-19；药物重定位;天然产物；芳香中药

1．前言

新型冠状病毒肺炎（COVID-19）的爆发使抗冠状病毒的药物研发再次成为世界瞩目的焦点，亟需筛选有效的药物来抵抗新型冠状病毒。回顾性研究发现，大量的 SARS 和 COVID-19 冠状病毒患者使用经验性的临床治疗策略，例如合成核苷类药物利巴韦林、激素药物皮质类固醇和的 I 型干扰素等药物，然而，这些药物的副作用非常严重（Yi et al 2004，Chen et al 2008，Yu et al 2012，Wanget al 2020）。2003 年在中国大陆 SARS 爆发时，约有 50％的患者除西药外还接受了的中草药作为辅助疗法，中西结合的方法对 SARS 患者产生了一些积极效果（Schwarz et al 2011）。

冠状病毒是一种有包膜的正向单链 RNA 病毒，典型的基因组大小约为 30kb，编码病毒 RNA 合成所需的非结构蛋白和结构蛋白，以及一些其他辅助蛋白（Roh et al 2012，Chiow et al 2016）。非结构蛋白包括 3-胰凝乳样蛋白酶(3-chymotrypsin-like protease，3CLpro)、木瓜样蛋白酶(Papain-like protease)、解旋酶(Helicase)、RNA 依赖性 RNA 聚合酶(RNA-dependent RNA polymerase，RdRp)，还包括刺突蛋白（S），包膜蛋白（E），膜蛋白（M）和核衣壳蛋白（N）(Li and De 2020)。在过去的十七年里，研究者们以冠状病毒的重要蛋白为靶标，探索了大量天然产物成分对冠状病毒的抑制活性；或者通过细胞实验直接验证小分子对冠状病毒侵染细胞活性的影响。

尽管研究者们认识到天然产物对冠状病毒治疗的重要性，并且已经发现了一部分活性较高的天然产物。但是直接通过体外实验从数目庞大的天然产物成分中筛选出有效的抗病毒成分仍然是一个工作量巨大的挑战。因此，运用药物重定位（老药新用）技术，通过计算工具快速筛选出最具潜力的天然产物再来进行实验验证，将会极大加快药物研发速度。

药物重定位被认为是最有前途的转化医学策略之一，药物重定位不仅能够使现有药物的价值得到更好的发挥，还可以避免药物 ADME/T 性质缺陷带来的药物研发失败（Wang and Zhang 2013）。寻找现有药物的新用途通常依赖于文本挖掘（Andronis et al 2011），化学遗传学（Iorioet al 2010）和网络分析（Dudley et al 2011）等方法。本文作者前期在重大新发传染病爆发期相关数据缺乏的情况下，提出了一种新的计算药理学方法，即 aCODE (agile discovery method of drugs or natural products for emerging epidemic)方法（全源等 2020）。该方法通过将有限疗效的广谱抗病毒药和部分报道有一定疗效提示的药物为输入，“钓鱼”获得其宿主靶蛋白集合，在全基因组尺度上搜索与之相关性最高的基因模块组合，进而对候选化合物进行模式匹配与统计检验排序，最后将初始药物与天然产物分子混合聚类，以了解候选化合物发挥作用的潜在细胞分子机制。

为了探讨 aCODE 方法在新冠病毒肺炎（COVID-19）天然产物计算筛选中的应用潜力，本文在 aCODE 1.0 基础上进行了数据扩充和算法约束，迭代更新为 aCODE 2.0 版本，优化了系统的精准度与预测能力。此外，本文以文献调研的方式综述了从 2003 年 SARS 爆发以来被证实有抗冠状病毒活性的天然产物成分的作用机制，并与 aCODE 平台所预测的天然产物进行证据集成，进一步探讨 aCODE 方法的应用价值。

2. 数据资源与分析方法

2.1 天然产物抗冠状病毒活性的文献调研

在本研究中，文献调研在谷歌学术上进行（https://f.glgoo.top/scholar），初始检索设定时间限制为“2003 年及以后”，关键词以“coronavirus”和“natural product”进行共显检索，选择前 20 篇文献精读记录，并以此 20 篇文献参考文献及引用文献中所涉及的天然产物为线索，整理一个具有抗冠状病毒活性的天然产物的初步

成分列表。随后进一步检索依次以"coronavirus+列表成分"进行遍历检索，从而对初步成分进行核减和扩充，扩充的新成分再次遍历，直至无新扩充天然产物成分为止。在文献检索过程中，凡综述中所述成分，应溯源其原始文献核实，核实不到的均予以核减。

全部天然产物成分按照其参考文献引用次数排序（Citations 列），有多篇文献的采用多篇 Citation 的总和进行的排序（Total 列）（附表 3）。

2.2 aCODE 系统数据与算法更新

在 aCODE 1.0 所运用的原基因模块（来源：Molecular Signatures Database（MSigDB）数据库（https://www.gsea-msigdb.org/gsea/msigdb/））的基础上，引入 STRING 数据库（https://string-db.org/）中的 PPI（Protein-Protein Interaction）信息拓展现有基因模块。

aCODE 基因模块更新后用于筛选药物的背景药物数据集来自天然产物（中药）化学成分数据库 Traditional Chinese Medicine Integrated Database（TCMID，http://www.megabionet.org/tcmid/）（Xue et al 2012）。

芳香植物成分计算数据来源为 AromaDb 数据库（http://bioinfo.cimap.res.in/aromadb/）（Yogesh et al 2018）。该数据库包括 1,321 种芳香化学结构，精油/芳香化合物的生物活性，357 种精油类型，166 种商用植物。芳香化合物作用于人体的靶标同样收集自 STITCH 数据库（Szklarczyk et al 2015），为了检索到具有不同靶标数量的化合物，分别设置参数 maxT（即允许每个候选化合物输入的 STITCH 靶标 CombinedScore 最高的 maxT 个靶基因）为 300、100。

aCODE 方法计算候选化合物靶基因与疾病相关模块基因集合交集的超几何分布检验 P 值，进而通过-log10(P)计算求和，得到候选化合物与疾病的相关性（全源等 2020），获得初始药物与天然产物（附表 2）及芳香成分（附表 4）的相关性列表。

3. 结果

3.1 冠状病毒靶标及其天然产物

自 2003 年 SARS 爆发以来，研究者们探索了数目庞大的天然产物成分对冠状病毒靶蛋白活性的影响。本文根据文献调研所得到的 56 个被实验证实有抗冠状病毒活性的天然产物成分，总结了针对几个重要的病毒靶标的天然产物成分及该靶标相对应的抗病毒药物（表 1）。

表 1.以冠状病毒蛋白为靶标的抗病毒药物及天然产物

药物靶标	中文名	抗病毒药	天然产物
Spike glycoprotein	S 蛋白	萘莫司他 Nafamostat（Manliet al 2007） 格瑞弗森 Griffithsin(O'Keefeet al 2007)	木犀草素 Luteolin（Ho et al 2007 ） 大黄素 Emodin（Yi et al 2004）
Nucleocapsid protein	N 蛋白	None	没食子儿茶素没食子酸酯 Gallocatechin gallate (Roh et al 2012) 白藜芦醇 Resveratrol (Linet al 2017)
3a protein	3a 蛋白	None	大黄素 Emodin (Schwarz et al 2011) 胡桃宁 Juglanin (Schwarz et al 2014)
3CLpro	3-胰凝乳样蛋白酶	洛匹那韦 Lopinavir（临床三期）(Sheahanet al 2020) 利托那韦 Ritonavir(临床三期) (Kimet al 2016)	橙皮素 Hesperetin (Lin et al 2005) 芦荟大黄素 Aloe emodin (Lin et al 2005) 槲皮素 Quercetin (Nguyen et al 2012) 单宁酸 Tannic acid (Chen et al 2005) 查尔酮 Chalcones (Park et al 2017) 草质素 Herbacetin (Jo et al 2019) 异补骨脂查尔酮 Isobavachalcone (Jo et al 2019)
Helicase	解旋酶	巴南宁 Bananins（临床前）(Zaheret al 2020) 三唑类化合物 Triazole derivatives (临床前) (Zaheret al 2020)	杨梅素 Myricetin (Yu et al 2012) 野黄芩素 Scutellarein (Yu et al 2012)
RdRp	RNA 依赖性 RNA 聚合酶	瑞德西韦 Remdesivir（临床三期）(Brown et al 2019) 法维拉韦 Favipiravir（随机临床）(Agostiniet al 2018)	None

注：所列药物及天然产物均为代表性分子

由表 1 可知，冠状病毒靶蛋白既可以是结构蛋白，比如刺突糖蛋白（Spike glycoprotein，S 蛋白）和核衣壳蛋白（Nucleocapsid protein，N 蛋白）；可以是非结构蛋白，比如 3-胰凝乳样蛋白酶(3CLpro)、解旋酶(Helicase)和 RNA 依赖性 RNA 聚合酶(RdRp)；也可以是其他的辅助蛋白，比如 3a 阳离子通道蛋白（3a 蛋白）。

3-胰凝乳样蛋白酶(3CLpro) 属于半胱氨酸蛋白酶，底物结合位点高度保守，是催化冠状病毒前体蛋白裂解的关键蛋白酶，用于病毒成熟期间的蛋白水解过程，对病毒的复制有重要作用，是目前广谱抗正向单链 RNA 病毒的重要靶点（Chen et al 2005，Nguyen et al 2012，Park et al 2017）。针对 3CLpro，Lin 等在 2005 年基于细胞的裂解试验检测了板蓝根提取物，5 种主要的靛蓝根化合物和 7 种植物

来源的酚类化合物的活性，最终筛选结果显示芦荟大黄素和橙皮素剂量依赖性地抑制了 3CLpro 的裂解活性。同样经过大量实验筛选出的具有抑制 3CLpro 活性的天然产物成分还有槲皮素、单宁酸、草质素、查尔酮、异补骨脂查耳酮等（Chen et al 2005，Nguyen et al 2012，Park et al 2017, Jo et al 2019）。

与 3CLpro 一同被关注的，还有病毒结构蛋白核衣壳蛋白(N)和刺突蛋白(S)，N 蛋白由于在冠状病毒复制中的重要作用，被视为抗 SARS 治疗的主要靶标，Roh 等在 2012 年通过设计生物芯片使用基于纳米颗粒的 RNA 寡核苷酸来分析 SARS-CoV N 蛋白的抑制剂，该实验证明了多酚化合物中儿茶素没食子酸酯和没食子儿茶素没食子酸酯具有显着的抑制活性（Roh et al. 2012）。S 蛋白抑制剂通过干扰 S 蛋白与宿主细胞的结合而起到抗病毒的作用，目前被证明有活性的天然产物成分为大黄素和木犀草素等。

另外一个有吸引力的靶标是冠状病毒开放阅读框 3a 蛋白形成的阳离子选择性通道，该通道可能在感染的细胞中表达，并参与病毒释放。抑制 3a 蛋白形成的离子通道的药物有望抑制病毒的释放，并且将成为开发新型治疗剂的来源（Schwarz et al 2011）。Schwarz 等人分别在 2011 和 2014 年证明了大黄素和胡桃宁对 3a 蛋白的抑制活性（Schwarz et al 2011，Schwarz et al 2014）。

研究者们除了探索以冠状病毒的重要蛋白为靶标的天然产物成分，也有大量研究通过如非洲绿猴肾细胞（Vero E6）的细胞实验直接验证小分子对冠状病毒复制的影响能力。比如，Wu 等人在 2004 年筛选的人参皂甙 Rb1、利血平、七叶皂苷等天然产物成分(Wu et al. 2004)，以及 Wen 等人在 2007 年证明有活性的柳杉酚、松柏酸和桦木酸等天然产物成分(Wen et al 2007)。

为了探讨 aCODE 方法在新冠病毒肺炎（COVID-19）天然产物计算筛选中的应用潜力，本文整理了所有具有抗冠状病毒活性的天然产物成分及其相关支持文献，汇总形成了 aCODE 计算所得中药天然产物（Tcm1，maxT=300，附表 1；Tcm2，maxT=100，附表 2)、以及有文献证据的抗冠状病毒的天然产物成分(表 2，附表 3)。

表 2.已有文献支持的 aCODE 平台计算所得的中药天然产物

Tcm1[a]	**中文名**	**Tcm2[b]**	**中文名**
Emodin	大黄素	Glycyrrhizin	甘草酸
Honokiol	和厚朴酚	Betulinic acid	桦木酸
Magnolol	厚朴酚	Quercitrin	槲皮苷
Myricetin	杨梅素	Myricetin	杨梅素
		Ginsenoside Rb1	人参皂甙 Rb1
		Reserpine	利血平

注：[a]maxT 参数设置为 300，偏重抓取靶标适中的化合物。

[b]maxT 参数设置为 100，偏重抓取靶标偏少的化合物。

表 2 中有两个天然产物非常值得关注，第一个是 Tcm1 中的大黄素(Emodin)，大黄素是 3a 蛋白(离子通道)的抑制剂，而且大黄素可能破坏 S 蛋白与宿主 ACE2 相互作用的发现，支持了大黄素或衍生物可能成为治疗 SARS 和其他冠状病毒引起的疾病的有效新治疗剂的建议（Ho et al 2007，Schwarz et al 2011）。第二个是 Tcm2 中的甘草酸，Cinatl 等在 2003 年评估了来自法兰克福大学临床中心的 SARS 患者的两种临床分离株冠状病毒（FFM-1 和 FFM-2）对利巴韦林、6-氮杂鸟苷、吡唑呋林、霉酚酸和甘草酸的抗病毒潜力，在所有化合物中，天然产物甘草酸在抑制 SARS 相关病毒复制的活性最强（Cinatl et al 2003）。并且许多甘草酸衍生物被证明具有较高的抗病毒生物活性（Wu et al 2004，Hoeveret al 2005，Chen et al 2008）。在最新的 COVID-19 药物研发中，甘草酸及其衍生物也是很多研究团队所重点关注的天然产物成分（Zhou et al 2020）。

除此之外，在本次新冠病毒肺炎（COVID-19）疫情中，丁虹等所提出的鸡尾酒疗法甘草酸方案（甘草酸+芦丁+维生素 C）已进入临床试验阶段。aCODE 预测结果同时涵盖了甘草酸、芦丁和维生素 C。

3.2 芳香成分抗冠状病毒活性预测及其潜在应用价值

Jasuja 等人在 2015 年提出很多植物精油(芳香类化合物)具有抗菌、抗氧化、抗病毒等活性，这些特性用于各种目的，包括治疗传染病(Jasujaet et al 2015)。在 2003 年 SARS 疫情之后，研究者们也加强了精油抗冠状病毒的活性研究，Loizzo 等人在 2008 年通过实验发现月桂精油（Laurus nobilis）对 SARS-CoV 具有有趣的活性，其 IC50 值为 120μg/ ml，选择性指数（SI）为 4.16，该精油的有效成分为 β-罗勒烯，1,8-桉树脑，α-松萜和 β-松萜(Jasujaet al 2008)。这说明芳香成分抗冠状病毒的应用潜力是值得被进一步挖掘的。

在前期发布的利用 aCODE 对中药天然产物的分析结果中，预测有效的化合物中出现了大量芳香化合物。本次更新中，我们增加了芳香植物提取物化学成分数据源，对芳香植物提取物的抗病毒活性进行了筛选(附表 4)。

由于对芳香提取物进行针对冠状病毒的研究相对较少，我们主要关注了 aCODE 结果中芳香化合物对病毒类广谱功效。例如，预测结果中的组氨酸（Histidine）具有抗艾滋病病毒活性（Dantas et al. 2019）。

除了组氨酸，在芳香成分预测结果中还发现了一些挥发性比较强芳香成分，如茴香烯、肉桂醛柠檬烯、芳樟醇、氨基肉桂酸。有趣的是在天然产物成分(Tcm)中也可以发现这些强挥发性的芳香成分，如水杨酸苄酯、紫苏醇、棕榈油酸和茴香烯。其中，肉桂酸和肉桂醛在很多研究中被报道具有抗病毒效应，例如 Vimalanathan 等在 2014 年报道了肉桂精油的蒸汽可能通过影响宿主的血凝素(HA)来影响流感病毒或其他呼吸类病毒的活性；Hayashi 等在 2007 年通过感染 A/PR/8 流感病毒的小鼠实验证明肉桂醛可以显著提高小鼠的存活率；Ding 等在 2011 年发现肉桂醛的代谢产物肉桂酸通过抑制宿主的 TLR4-NF-κB 信号转导途径直接减轻了由柯萨奇病毒 B3（CVB3）诱导的病毒性心肌炎（VMC）中的炎

症反应；Gravina 等在 2011 年通过体外实验证明肉桂酸具有影响马疱疹病毒 1（EHV-1）复制周期的活性。另外，Choi 等人在 2018 年通过对 11 种精油检测其抗流感病毒效果发现，多种含有芳樟醇的精油可减少甲型流感/ WS/33 病毒导致的细胞病理效应，具有潜在抗甲型流感/WS/33 病毒的作用。

以上结果强烈提示这些芳香化合物具有潜在的抗冠状病毒活性和开发应用价值。除此之外，大多数抗病毒文献是以精油为单位研究，没有针对芳香植物中具体有效化学成分进行抗病毒活性分析。因此，在针对天然产物/精油的药物研发过程中，明确其真正有效的化学成分将是一个重要的发展趋势。

4. 讨论

本文通过将 aCODE 计算药理学结果与文献综述进行比对分析，发现部分候选化合物经过实验验证被发现有抗冠状病毒的活性。尽管研究者们认识到天然产物对冠状病毒治疗的重要性，但是传统方式试图从数目庞大的天然产物分子库中通过实验来筛选出有效的抗病毒成分，筛选范围十分有限且效率不高，导致很多有潜力的天然产物成分不能够被及时发现。因此，本文作者所提出的 aCODE 老药新用计算平台为高效的天然产物抗冠状病毒活性开发提供了技术支持，将会大幅度的节约提出科学假说的时间。尤其是对中药天然产物、对药食同源成分的分析，将有助于提出安全性高、副作用顾虑比较小的防治方案。

一般认为中药天然产物主要靶向宿主，而对病毒的直接作用比较少。本次计算与文献证据的集成分析，提示可能存在一个新的规律，即中药天然产物不光可以调节人体状态，也可以全面靶向病毒、靶向病毒-宿主相互作用的各个环节，是一个不可忽视的因素。当前，在新冠肺炎临床实践中，靶向病毒、靶向宿主双管齐下，在不同阶段综合考虑控制病毒、调节宿主反应（例如炎症风暴）与器官功能维护，是一个重要的发展趋势。中药天然产物有潜力在疾病防治各阶段均发挥重要作用。

尤其值得关注的是，四大文明古国均有使用芳香植物对抗瘟疫的大量报道。在中国传统医学中，芳香植物在历次大瘟疫中被广泛使用于预防、治疗等环节。“芳香避秽”，除了预防，能否在病毒及其与宿主的相互作用过程中发挥作用？大部分药物受阻于血脑屏障不能进入脑组织而对某些中枢神经损伤望洋兴叹，能否利用芳香产物的优势加强脑损伤保护？由于古代制剂技术的限制，芳香类化合物在中药煎煮过程中很容易挥发，因此芳香中药在中国传统医学中没有得到足够的重视。随着现代生物制剂技术的进步，芳香中药的科学化，将在重大传染病防治中发挥更重要的作用。另外如何利用化学分析、植物代谢组学、表观遗传学、计算药理学降低芳香中药应用中的不确定性，将是后续的重点研究方向。

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附表 1. COVID-19 药物与天然产物（中药）来源的候选化合物及其分子机制

Compound name	名称	类型	相关性	显著关联基因模块（Top 3）
DEOXYCHOLICACID	脱氧胆酸	T	1182	ppi_STAT3, ppi_STAT5B, ppi_TP53, ppi_JUN, ppi_MMP9
BENZENE	苯	T	1150	ppi_STAT5A, ppi_AKT1, ppi_STAT3, ppi_MYC, ppi_TP53
APIGENIN	芹菜素	T	1141	ppi_CCND2, ppi_STAT5A, ppi_STAT3, ppi_STAT5B, ppi_MYC
SILICON DIOXIDE	二氧化硅	T	1137	ppi_AKT1, ppi_STAT3, ppi_MYC, ppi_JUN, ppi_MMP9
1-METHOXYCANTHIN-6-ONE	1-甲氧嘧啶-6-1	T	1111	ppi_CCND2, ppi_STAT5A, ppi_AKT1, ppi_STAT3, ppi_STAT5B
3,4-BENZOPYRENE	3,4-苯并芘	T	1111	ppi_AKT1, ppi_MYC, ppi_TP53, ppi_JUN, ppi_MCL1
2-PROPENAL	2-丙烯醛	T	1075	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, ppi_TP53, ppi_FOS, ppi_MCL1
BAICALEIN	黄芩素	T	1038	ppi_STAT3, ppi_MYC, ppi_TP53, ppi_JUN, ppi_FOS
CHLOROQUINE	氯喹	D	1016	ppi_STAT5A, ppi_AKT1, ppi_STAT3, ppi_STAT5B, ppi_MYC
4-METHYLSULFINYL BUTYL ISOTHIOCYANATE	4-甲基亚磺酰基丁基异硫氰酸酯	T	974	ppi_CCND2, ppi_MYC, ppi_TP53, ppi_JUN, ppi_FOS
SULFORATHANE	磺胺硫烷	T	974	ppi_CCND2, ppi_MYC, ppi_TP53, ppi_JUN, ppi_FOS
DIHYDROTESTOSTERONE	二氢睾酮	T	890	ppi_SRC, ppi_CREB1, ppi_SP1, ppi_ESR1, ppi_EGR1
RIBAVIRIN	利巴韦林	D	848	ppi_STAT5A, ppi_STAT3, ppi_STAT5B, ppi_LCK, ppi_FOS
BERBERINE	小檗碱	T	836	ppi_NEURL1, ppi_NEURL1B, ppi_JUN, ppi_NFKB1, ppi_PTPN1
1,7-DIPHENYL-5-HEPTENE-3-ONE	1,7-二苯基-5-庚烯-3-1	T	830	ppi_CCND2, ppi_STAT5A, ppi_AKT1, ppi_STAT3, ppi_STAT5B
1,7-DIPHENYLHEPT-4-EN-3-ONE	1,7-二苯甲基-4-EN-3-1	T	830	ppi_CCND2, ppi_STAT5A, ppi_AKT1, ppi_STAT3, ppi_STAT5B
BENZYL SALICYLATE	水杨酸苄酯	T	830	ppi_CCND2, ppi_STAT5A, ppi_AKT1, ppi_STAT3, ppi_STAT5B
RITONAVIR	利托那韦	D	767	ppi_CCND2, ppi_NEURL1, ppi_NEURL1B, ppi_TP53, ppi_CDK5
ANTHRACENE	蒽	T	765	ppi_AR, ppi_TP53, ppi_NRAS, ppi_JUN, ppi_KRAS
KAEMPFEROL	山柰酚	T	753	ppi_JUN, ppi_NFKB1, ppi_TP53, ppi_FOS, ppi_ESR1
L-HOMOCYSTEINE	同型半胱氨酸	T	752	ppi_AKT1, ppi_JUN, ppi_MMP9, ppi_SRC, ppi_NFKB1
FUMARICACID	富马酸	T	725	ppi_STAT5A, ppi_STAT3, ppi_STAT5B, ppi_PTEN, ppi_GRB2
EMODIN	大黄素	T	674	ppi_TP53, ppi_JUN, ppi_FOS, ppi_ESR1, ppi_NFKB1
ARECOLINE	槟榔碱	T	637	ppi_MMP9, ppi_STAT3, ppi_TP53, ppi_JUN, ppi_NFKB1
4-(1-METHYLETHENYL)-1-CYCLOHEXENE-1-METHANOL	4-(1-甲基乙烯基)-1-环己烯-1-甲醇	T	632	ppi_SNAI1, ppi_WWOX, ppi_LCK, ppi_NRAS, ppi_NFKB1
PERILLA ALCOHOL	紫苏醇	T	632	ppi_SNAI1, ppi_WWOX, ppi_LCK, ppi_NRAS, ppi_NFKB1
PERILLYL ALCOHOL	紫苏醇	T	632	ppi_SNAI1, ppi_WWOX, ppi_LCK, ppi_NRAS, ppi_NFKB1
ATENOLOL	阿替洛尔	T	614	ppi_STAT5A, ppi_STAT3, ppi_STAT5B, ppi_FOS, ppi_SRC
3,4,5-TRIHYDROXYBENZOIC ACID	3,4,5-三羟基苯甲酸	T	612	ppi_BAX, ppi_NFKB1, ppi_CDH1, ppi_MCL1, ppi_HBEGF
GALLICACID	没食子酸	T	612	ppi_BAX, ppi_NFKB1, ppi_CDH1, ppi_MCL1, ppi_HBEGF
ZERUMBONE	蛇骨	T	609	ppi_HRAS, ppi_NFKB1, ppi_MCL1, ppi_RAC1, ppi_STAT3
PALMITOLEICACID	棕榈油酸	T	574	ppi_STAT5A, ppi_STAT3, ppi_STAT5B, ppi_PTEN, GO_PROTEIN_TYROSINE_KINASE_ACTIVITY
L-ALPHA,GAMMA-DIAMINOBUTYRIC ACID	l-α,γ-二氨基丁酸	T	571	ppi_STAT5A, ppi_STAT3, ppi_STAT5B, ppi_PTEN, ppi_GRB2
ECKOL	鹅掌菜酚	T	567	KEGG_ERBB_SIGNALING_PATHWAY, ppi_KRAS, ppi_NRAS, ppi_MDK, ppi_NFKB1
PHENETHYL CAFFEATE	咖啡酸苯乙酯	T	561	ppi_ESR2, KEGG_NON_SMALL_CELL_LUNG_CANCER, ppi_PTPN1, ppi_CDH17, ppi_MMP9
NORDIHYDROGUAIARETICACID	去甲二氢愈创木酸	T	553	ppi_FOS, ppi_SRC, ppi_FGF2, ppi_MMP9, ppi_EGR1
THREONINE	苏氨酸	T	549	ppi_CCND1, ppi_SNCA, ppi_TOP2A, ppi_PRKN, ppi_CREB1

CALCIUM PHOSPHATE	磷酸钙	T	531	ppi_SMAD2, ppi_MMP9, ppi_EGR1, ppi_SNAI1, ppi_JUN
HYDROXYBENZENE	酚	T	531	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, ppi_FOS, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, ppi_BAX
PHENOL	苯酚	T	531	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, ppi_FOS, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, ppi_BAX
PHENYLIC ACID	苯甲酸	T	531	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, ppi_FOS, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, ppi_BAX
WOGONIN	沃贡宁	T	530	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, ppi_MAPK3, ppi_RHOA, ppi_MAPK1
FISETIN	非瑟汀	T	504	ppi_RGCC, ppi_TOP2A, ppi_NFKB1, KEGG_NON_SMALL_CELL_LUNG_CANCER, ppi_JUN
DIBUTYL PHTHALATE	邻苯二甲酸二丁酯	T	503	ppi_PTPN1, ppi_NFKB1, ppi_AR, ppi_MAPK1, ppi_SP1
PTEROSTILBENE	蕨类植物	T	496	ppi_JUN, ppi_NFKB1, ppi_BAX, ppi_FOS, ppi_MCL1
MAGNOLOL	厚朴酚	T	492	ppi_FGF7, ppi_MMP9, ppi_FGF2, ppi_NFKB1, ppi_AR
ALLITRIDIN	大蒜素	T	491	ppi_NFKB1, ppi_FOS, ppi_EGFR, ppi_PRKN, ppi_HRAS
DIALLYL TRISULFIDE	二硫化三烯丙基	T	491	ppi_NFKB1, ppi_FOS, ppi_EGFR, ppi_PRKN, ppi_HRAS
3BETA-HYDROXY-ANDROST-5-ENE-17-ONE	3-B-羟基-去氧雄甾-5-烯-17-酮-3	T	486	ppi_FOS, ppi_AR, ppi_ESR1, ppi_MMP9, ppi_EGR1
SILICON	硅	T	476	ppi_TF, ppi_FOS, ppi_ESR1, ppi_HRAS, ppi_RHOA
NEOISORUTIN	新异芦丁	T	466	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_MELANOMA, REACTOME_NEGATIVE_REGULATION_OF_THE_PI3K_AKT_NETWORK, ppi_MYOD1
RUTIN	芦丁	T	466	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_MELANOMA, REACTOME_NEGATIVE_REGULATION_OF_THE_PI3K_AKT_NETWORK, ppi_MYOD1
VITAMIN P	维生素 P	T	466	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_MELANOMA, REACTOME_NEGATIVE_REGULATION_OF_THE_PI3K_AKT_NETWORK, ppi_MYOD1
URACIL	尿嘧啶	T	465	ppi_TOP2A, ppi_GMPS, ppi_TOP2B, ppi_TP53, ppi_ERBB3
NELFINAVIR	奈非那韦	D	465	ppi_NEURL1, ppi_NEURL1B, ppi_AKT1, ppi_STAT3, ppi_TP53
ASCORBIC ACID	抗坏血酸	T	462	GO_COFACTOR_METABOLIC_PROCESS, ppi_JUN, ppi_MYC, ppi_MMP9, ppi_MT-CYB
VITAMIN C	维生素 C	T	462	GO_COFACTOR_METABOLIC_PROCESS, ppi_JUN, ppi_MYC, ppi_MMP9, ppi_MT-CYB
1-METHOXY-4-(1-PROPENYL)-BENZENE	1-甲氧基-4-(1-丙烯基)-苯	T	453	ppi_NFKB1, ppi_SNAI1, ppi_PTEN, KEGG_CHRONIC_MYELOID_LEUKEMIA, KEGG_MELANOMA
1-METHOXY-4-(1-PROPENYL)BENZENE	1-甲氧基-4-(1-丙烯基)苯	T	453	ppi_NFKB1, ppi_SNAI1, ppi_PTEN, KEGG_CHRONIC_MYELOID_LEUKEMIA, KEGG_MELANOMA
ANETHOLE	茴香烯	T	453	ppi_NFKB1, ppi_SNAI1, ppi_PTEN, KEGG_CHRONIC_MYELOID_LEUKEMIA, KEGG_MELANOMA
CIS-ANETHOLE	顺式茴香烯	T	453	ppi_NFKB1, ppi_SNAI1, ppi_PTEN, KEGG_CHRONIC_MYELOID_LEUKEMIA, KEGG_MELANOMA
P-PROPENYL-ANISOLE	对丙烯基茴香醚	T	453	ppi_NFKB1, ppi_SNAI1, ppi_PTEN, KEGG_CHRONIC_MYELOID_LEUKEMIA, KEGG_MELANOMA
TRANS-ANETHOLE	反式茴香烯	T	453	ppi_NFKB1, ppi_SNAI1, ppi_PTEN, KEGG_CHRONIC_MYELOID_LEUKEMIA, KEGG_MELANOMA
DELPHINIDIN	翠雀素	T	452	ppi_TP53, ppi_JUN, ppi_STAT5A, ppi_FOS, ppi_NFKB1
ALIZARIN	茜素	T	435	ppi_FGF7, ppi_SMAD2, ppi_SNAI1, ppi_FGF2, ppi_EGR1
CREATININE	肌酐	T	420	ppi_MMP9, ppi_JUN, ppi_AKT1, ppi_FGF2, ppi_NFKB1
ELLIPTICINE	玫瑰树碱	T	412	ppi_MCL1, KEGG_P53_SIGNALING_PATHWAY, ppi_BAX, GO_DNA_CONFORMATION_CHANGE, ppi_TP53
COMPOUND 5	化合物 5	T	410	ppi_PPIG, ppi_TNK2, GO_UNFOLDED_PROTEIN_BINDING, ppi_STAT5B, ppi_STAT3
3,3',4',5,5',7-HEXAHYDROXYFLAVONE	3,3',4',5,5',7-六羟基黄酮	T	409	ppi_AKT1, ppi_NRAS, ppi_PIK3R3, ppi_HRAS, KEGG_NON_SMALL_CELL_LUNG_CANCER
MYRICETIN	杨梅素	T	409	ppi_AKT1, ppi_NRAS, ppi_PIK3R3, ppi_HRAS, KEGG_NON_SMALL_CELL_LUNG_CANCER

PYRIDINE	吡啶	T	407	ppi_JUN, ppi_BAX, ppi_FOS, ppi_CREB1, ppi_MCL1
METHYLBENZENE	甲苯	T	405	ppi_FOS, ppi_JUN, GO_DRUG_METABOLIC_PROCESS, ppi_AKT1, ppi_CREB1
METHYLBENZOL	甲基苯甲	T	405	ppi_FOS, ppi_JUN, GO_DRUG_METABOLIC_PROCESS, ppi_AKT1, ppi_CREB1
TOLUENE	甲苯	T	405	ppi_FOS, ppi_JUN, GO_DRUG_METABOLIC_PROCESS, ppi_AKT1, ppi_CREB1
PONASTERONE A	脱皮素甲	T	392	ppi_ESR1, ppi_AR, ppi_ESR2, ppi_NR4A2, ppi_NCOR1
HONOKIOL	厚朴酚	T	390	GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, GO_ENDOPEPTIDASE_ACTIVITY, ppi_BAX, ppi_RHOA
OCTADECANOIC ACID	十八烷酸	T	383	ppi_ESR1, ppi_AR, ppi_ESR2, ppi_NR4A2, ppi_NCOR1
STEARICACID	硬脂酸	T	383	ppi_ESR1, ppi_AR, ppi_ESR2, ppi_NR4A2, ppi_NCOR1
ALPHA-ALLOKAINIC ACID	α-链烷酸	T	372	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, ppi_FOS, ppi_CREB1, ppi_NTRK2
KAINIC ACID	海藻酸	T	372	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, ppi_FOS, ppi_CREB1, ppi_NTRK2
BENZYL ISOTHIOCYANATE	异硫氰酸苄酯	T	360	ppi_EPCAM, ppi_ESR2, ppi_CDH17, ppi_MMP9, ppi_EGFR
NICOTINAMIDE	烟酰胺	T	360	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, ppi_AKT1, ppi_EDDM3B
VITAMIN B	维生素 b	T	360	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, ppi_AKT1, ppi_EDDM3B
DIHYDROCAPSAICIN	二氢辣椒素	T	360	ppi_MCL1, KEGG_NON_SMALL_CELL_LUNG_CANCER, ppi_PRKCD, GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, KEGG_GLIOMA
ALPHA-D-FRUCTOFURANOSE	α-d-果糖呋喃糖	T	359	ppi_AKT1, ppi_CREB1, ppi_TF, ppi_MYC, ppi_TOP2A
BETA-D-FRUCTOFURANOSE	β-d-果糖呋喃糖	T	359	ppi_AKT1, ppi_CREB1, ppi_TF, ppi_MYC, ppi_TOP2A
FRUCTOSE	果糖	T	359	ppi_AKT1, ppi_CREB1, ppi_TF, ppi_MYC, ppi_TOP2A
STEROL	固醇	T	356	ppi_ESR1, ppi_CREB1, ppi_SP1, ppi_NCOR1, GO_COFACTOR_METABOLIC_PROCESS
PYRENE	芘	T	355	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, GNF2_HPX, HSIAO_LIVER_SPECIFIC_GENES
ESTRONE	雌酮	T	352	GO_DRUG_METABOLIC_PROCESS, ppi_PPIG, ppi_ESR1, ppi_EGR1, ppi_FOS
OESTRONE	雌酮	T	352	GO_DRUG_METABOLIC_PROCESS, ppi_PPIG, ppi_ESR1, ppi_EGR1, ppi_FOS
PICEATANNOL	苦味酚	T	351	GO_PROTEIN_TYROSINE_KINASE_ACTIVITY, ppi_JUN, ppi_CREB1, ppi_KRAS, ppi_MMP9
3,5,3'-TRIIODOTHYRONINE	3,5,3'-三碘甲状腺素	T	349	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, ppi_AR, ppi_ESR2, ppi_NR4A2
LOPINAVIR	洛匹那韦	D	341	ppi_PTPN1, ppi_SRC, ppi_LCK, GO_ENDOPEPTIDASE_ACTIVITY, ppi_HBEGF
3-BUTYLIDENE PHTHALIDE	3-亚丁基苯酞	T	340	KEGG_P53_SIGNALING_PATHWAY, ppi_BAX, ppi_MCL1, KEGG_NON_SMALL_CELL_LUNG_CANCER, GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY
3-BUTYLIDENE-PHTHALIDE	3-丁叉苯	T	340	KEGG_P53_SIGNALING_PATHWAY, ppi_BAX, ppi_MCL1, KEGG_NON_SMALL_CELL_LUNG_CANCER, GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY
BUTYLIDENEPHTHALIDE	丁二烯	T	340	KEGG_P53_SIGNALING_PATHWAY, ppi_BAX, ppi_MCL1, KEGG_NON_SMALL_CELL_LUNG_CANCER, GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY
E-BUTYLIDENEPHTHALIDE	丁二烯	T	340	KEGG_P53_SIGNALING_PATHWAY, ppi_BAX, ppi_MCL1, KEGG_NON_SMALL_CELL_LUNG_CANCER, GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY
N-BUTYLIDENE PHTHALIDE	正丁烯酞	T	340	KEGG_P53_SIGNALING_PATHWAY, ppi_BAX, ppi_MCL1, KEGG_NON_SMALL_CELL_LUNG_CANCER, GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY
(+)-CATECHIN	(+)-儿茶素	T	335	ppi_HBEGF, ppi_FOS, ppi_NFKB1, ppi_MMP14, ppi_MMP9

注："类型"栏标注"D"表示该化合物为初始输入药物，"T"表示天然产物（中药）成分。

附表 2.　COVID-19 药物与天然产物（中药）来源的候选化合物及其分子机制

Compound name	名称	类型	相关性	显著关联基因模块（Top 5）	植物来源
DAIDZEIN	黄豆苷元	T	893.9966	STAT3_subnet, TP53_subnet, NFKB1_subnet, STAT5A_subnet, FOS_subnet	山豆根,豆油,淡豆豉,黑大豆,葛蔓,三消草,葛谷,红车轴草,黄大豆,苜蓿,葛花,鸡血藤,葛根,葛叶
BAICALEIN	黄芩素	T	835.4736	STAT3_subnet, TP53_subnet, NFKB1_subnet, FOS_subnet, PTEN_subnet	木蝴蝶,车前子,黄苓,车前,大车前,木瑚蝶树皮,车前草,黄芩,黄芩子
RITONAVIR	利托那韦	D	642.0844	STAT3_subnet, TP53_subnet, NFKB1_subnet, AKT1_subnet, STAT5A_subnet	
LYCOPENE	番茄红素	T	503.3181	TP53_subnet, MMP9_subnet, EGR1_subnet, FGF2_subnet, MYC_subnet	番茄,柿蒂,南鹤虱
ARECOLINE	槟榔碱	T	450.4329	MMP9_subnet, STAT3_subnet, TP53_subnet, JUN_subnet, NFKB1_subnet	槟榔,焦槟榔,大附皮
NELFINAVIR	奈非那韦	D	409.9464	GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, TP53_subnet, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, AR_subnet, AKT1_subnet	
NORDIHYDROGUAIARETICACID	去甲二氢愈创木酸	T	404.584	FOS_subnet, SRC_subnet, FGF2_subnet, MMP9_subnet, EGR1_subnet	五味子
3,4,5-TRIHYDROXYBENZOIC ACID	3,4,5-三羟基苯甲酸	T	390.9928	BAX_subnet, NFKB1_subnet, CDH1_subnet, MCL1_subnet, HBEGF_subnet	大黄茎,大黄
GALLICACID	没食子酸	T	390.9928	BAX_subnet, NFKB1_subnet, CDH1_subnet, MCL1_subnet, HBEGF_subnet	月季花,鹿衔草,油柑叶,棕榈皮,玫瑰花,黄连芽,柿蒂,红筷子,胡桃叶,白芍,马桑叶,醋柳果,虎杖,委陵菜,苏木,牵牛子,仙鹤草,拳参,继木,牡丹皮,白花前胡,地榆,山茱萸,大黄,相思子,葩蓄,柽柳,杨梅树皮,朮果,地锦草,诃子,白蔹,石榴皮,葫芦巴
ISOFLAVONE	异黄酮	T	384.3733	NFKB1_subnet, STAT5A_subnet, AKT1_subnet, STAT5B_subnet, JUN_subnet	豆豉,大黄豆卷,黑豆,焦三仙,新豉
CHLOROQUINE	氯喹	D	382.7235	AKT1_subnet, NFKB1_subnet, SRC_subnet, MMP9_subnet, TP53_subnet	
BUFALIN	蟾酥灵	T	378.801	SMAD2_subnet, BMP4_subnet, NFATC1_subnet, NFKB1_subnet, SP1_subnet	蟾酥
L20	l20	T	368.99	PTEN_subnet,	

				GO_PROTEIN_AUTOPHOSPHORYLATION, GLI1_subnet, MCL1_subnet, RAC1_subnet	
NARINGIN	柚皮苷	T	365.0071	JUN_subnet, FOS_subnet, NFATC1_subnet, CREB1_subnet, EGR1_subnet	柠檬,柠檬皮,枳实,枳壳,骨碎补,千斤拔,橘皮,枳壳,炒枳壳,炒神曲,化橘红
BETULIC ACID	丁二酸	T	352.4297	JUN_subnet, TFDP2_subnet, RGCC_subnet, FGF2_subnet, BAX_subnet	木槿皮,柿蒂,马通
BETULINIC ACID	桦木酸	T	352.4297	JUN_subnet, TFDP2_subnet, RGCC_subnet, FGF2_subnet, BAX_subnet	连翘,枣仁,炒枣仁,酸枣仁,三棱,大枣
PONASTERONE A	百日青蜕皮酮 A	T	349.6239	ESR1_subnet, AR_subnet, ESR2_subnet, NCOR1_subnet, SRC_subnet	紫杉,小叶贯众
ALIZARIN	茜草素	T	319.9601	BMP4_subnet, SMAD2_subnet, SNAI1_subnet, FGF2_subnet, EGR1_subnet	五爪龙,茜草
PLUMBAGIN	白花丹素	T	306.3735	MYC_subnet, MCL1_subnet, RUNX3_subnet, TP53_subnet, CREB1_subnet	白花丹,茅膏菜,紫雪花
NOVOBIOCIN	新霉素	T	304.5525	HSP90AB1_subnet, RGCC_subnet, TK2_subnet, TFDP2_subnet, E2F4_subnet	马钱子
RIBAVIRIN	利巴韦林	D	297.2476	LCK_subnet, STAT3_subnet, NFKB1_subnet, STAT5A_subnet, EGR1_subnet	
PUERARIN	葛根素	T	294.2354	MCL1_subnet, JUN_subnet, BAX_subnet, GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, NFKB1_subnet	甘葛藤根,葛根
FISETIN	非瑟酮	T	292.4296	RGCC_subnet, TOP2A_subnet, NFKB1_subnet, JUN_subnet, MCL1_subnet	黄连芽,儿茶,孩儿茶,朮果
ALLITRIDIN	大蒜素	T	273.2033	NFKB1_subnet, FOS_subnet, EGFR_subnet, PRKN_subnet, TP53_subnet	大蒜
DIALLYL TRISULFIDE	二硫化三烯丙基	T	273.2033	NFKB1_subnet, FOS_subnet, EGFR_subnet, PRKN_subnet, TP53_subnet	大蒜
APICIDIN	阿匹西丁	T	266.6731	NCOR1_subnet, MCL1_subnet, BCL6_subnet, RUNX3_subnet, NFKB1_subnet	浙贝母
ICARIIN	苦瓜素	T	256.0318	ESR1_subnet, AR_subnet, ESR2_subnet, NCOR1_subnet, SRC_subnet	仙灵脾,淫羊霍
3,3',4',5,5',7-HEXAHYDROXYFLAVONE	3,3'，4'，5,5'，7-六羟基黄酮	T	237.2842	AKT1_subnet, NRAS_subnet, PIK3R3_subnet, HRAS_subnet, PTEN_subnet	路路通,风箱树根,白胶香,风箱树叶,枫香树皮
MYRICETIN	杨梅素	T	237.2842	AKT1_subnet, NRAS_subnet, PIK3R3_subnet, HRAS_subnet, PTEN_subnet	显齿蛇葡萄,杨梅,银杏叶,侧柏叶,醋柳果,杨梅核仁,杨梅根,柏枝节,五倍子,鬼箭锦鸡儿,白花映山红,无莿根,杨梅树皮,柏根白皮

(+)-ARTEANNUIN	(+) -青蒿素	T	225.2435	JUN_subnet, TP53_subnet, PTPN1_subnet, MCL1_subnet, FOS_subnet	黄花蒿
ARTEANNUIN	青花蒿素	T	225.2435	JUN_subnet, TP53_subnet, PTPN1_subnet, MCL1_subnet, FOS_subnet	黄花蒿,黄蒿
ARTEMISININ	青蒿素	T	225.2435	JUN_subnet, TP53_subnet, PTPN1_subnet, MCL1_subnet, FOS_subnet	黄花蒿
(+)-CATECHIN	(+) -儿茶素	T	210.2609	HBEGF_subnet, NFKB1_subnet, BAX_subnet, FOS_subnet, MMP14_subnet	赤芍,茶叶,棕榈皮,银杏叶,槟榔,昆明山海棠,罗布麻,白芍,醋柳果,虎杖,仙鹤草,牛西西,桃仁,孩儿茶,白果,毛果芍药,大枣
(-)-CATECHIN	(-)-儿茶素	T	210.2609	HBEGF_subnet, NFKB1_subnet, BAX_subnet, FOS_subnet, MMP14_subnet	赤芍,银杏叶,白芍,毛果芍药
(-)-EPICATECHIN	(-)-表儿茶素	T	210.2609	HBEGF_subnet, NFKB1_subnet, BAX_subnet, FOS_subnet, MMP14_subnet	土茯苓
ALPHA-CATECHIN	α-儿茶素	T	210.2609	HBEGF_subnet, NFKB1_subnet, BAX_subnet, FOS_subnet, MMP14_subnet	满山红油
CATECHIN	儿茶素	T	210.2609	HBEGF_subnet, NFKB1_subnet, BAX_subnet, FOS_subnet, MMP14_subnet	赤芍,茶叶,银杏叶,绿茶,白芍,毛果芍药
D-CATECHIN	d-儿茶素	T	210.2609	HBEGF_subnet, NFKB1_subnet, BAX_subnet, FOS_subnet, MMP14_subnet	明党参,白芍,拳参,小甘草,党参芦头
EPICATECHIN	表儿茶素	T	210.2609	HBEGF_subnet, NFKB1_subnet, BAX_subnet, FOS_subnet, MMP14_subnet	白果叶,茶叶,土茯苓,贯叶连翘,山楂,越橘叶,拳参,孩儿茶,大黄,白果
MYCOPHENOLATE MOFETIL	霉酚酸酯	D	209.851	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, GO_HUMORAL_IMMUNE_RESPONSE, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, REACTOME_COMPLEMENT_CASCADE	
CINNAMALDEHYDE	肉桂醛	T	208.7601	FOS_subnet, JUN_subnet, PTPN1_subnet, NFKB1_subnet, MMP9_subnet	除虫菊,桂皮,桂子,桂皮油,桂丁,肉桂叶,桂枝,没药,广藿香油,广藿香叶,制没药,肉桂,广霍香
CINNAMIC ALDEHYDE	肉桂醛	T	208.7601	FOS_subnet, JUN_subnet, PTPN1_subnet, NFKB1_subnet, MMP9_subnet	狼毒,桂枝,肉桂
EVODIAMINE	乙二胺	T	206.311	MCL1_subnet, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, JUN_subnet, BAX_subnet	毛脉吴茱萸,吴茱萸根,吴茱萸叶,吴芋,少果吴茱萸,吴茱萸
ISOEVODIAMINE	异戊二胺	T	206.311	MCL1_subnet, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY,	吴茱萸

INDOLE	吲哚	T	205.7058	GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, JUN_subnet, BAX_subnet FOS_subnet, MMP9_subnet, EGR1_subnet, ESR1_subnet, CREB1_subnet	灵猫香,茶叶,白玉兰,板蓝根,白兰花
PERIDININ	苦瓜素	T	182.6642	RPL5_subnet, TOP2B_subnet, TOP2A_subnet, SRC_subnet, YES1_subnet	
2,6-DITERTBUTYL-4-METHYLPHENOL	2,6-二叔丁基-4-甲基苯酚	T	168.7569	GO_D_METABOLIC_PROCESS, GO_COFACTOR_METABOLIC_PROCESS, SRC_subnet, HSIAO_LIVER_SPECIFIC_GENES, ESR1_subnet	三七,西洋参,人参
BUTYLATED HYDROXYTOLUENE	丁基羟基甲苯	T	168.7569	GO_D_METABOLIC_PROCESS, GO_COFACTOR_METABOLIC_PROCESS, SRC_subnet, HSIAO_LIVER_SPECIFIC_GENES, ESR1_subnet	喜树皮,喜树叶,喜树,漏芦
GINSENOSIDE RB1	人参皂苷rb1	T	165.8182	ANGPT2_subnet, JUN_subnet, PTPN1_subnet, GO_COFACTOR_METABOLIC_PROCESS, FOS_subnet	汉三七,三七,人参,红参
GINSENOSIDE RBL	人参皂苷	T	165.8182	ANGPT2_subnet, JUN_subnet, PTPN1_subnet, GO_COFACTOR_METABOLIC_PROCESS, FOS_subnet	汉三七
FOLINIC ACID	亚叶酸	T	164.8792	TOP2A_subnet, GO_D_METABOLIC_PROCESS, TOP2B_subnet, HBEGF_subnet, MOOTHA_MITOCHONDRIA	荔枝,东当归,桑叶,人参,醋柳果,红车轴草,菠菜,川芎,黄芪,朮果
BENZYL ISOTHIOCYANATE	异硫氰酸苄酯	T	154.8658	ESR2_subnet, MYC_subnet, EGFR_subnet, NFKB1_subnet, MMP9_subnet	芥子,旱莲花,葶苈子,番木瓜
BUTEIN	紫铆因	T	152.1405	GO_D_METABOLIC_PROCESS, GO_COFACTOR_METABOLIC_PROCESS, MMP9_subnet, KRAS_subnet, MMP14_subnet	杞子,葎草,墨旱莲
INDINAVIR	茚地那韦	D	149.8173	GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, STAT5B_subnet, STAT3_subnet, AKT1_subnet	
N-METHYLPHENYLALANINE	正甲基苯丙氨酸	T	147.0078	GTPBP4_subnet, RPL5_subnet, FBL_subnet, NIP7_subnet, GMPS_subnet	
ALGINIC ACID	海藻酸	T	146.964	SMAD2_subnet, MMP9_subnet, GO_REGULATION_OF_VASCULATURE	昆布,海藻

				_DEVELOPMENT, TF_subnet, FGF2_subnet	
2,6,10,14-TETRAMETHYL PENTADECANE	2,6,10,14-四甲基十五烷	T	145.1185	STAT3_subnet, NFKB1_subnet, CD44_subnet, GO_ADAPTIVE_IMMUNE_RESPONSE_BASED_ON_SOMATIC_RECOMBINATION_OF_IMMUNE_RECEPTORS_BUILT_FROM_IMMUNOGLOBULIN_SUPERFAMILY_DOMAINS, STAT5A_subnet	威灵仙,灵仙
PICROPODOPHYLLIN	鬼臼苦素	T	142.2824	CDK5_subnet, HSP90AB1_subnet, AKT1_subnet, ESR1_subnet, MYC_subnet	盾叶鬼臼,鬼臼,窝儿七,浙贝母,山荷叶
PODOPHYLLOTOXIN	足叶草毒素	T	142.2824	CDK5_subnet, HSP90AB1_subnet, AKT1_subnet, ESR1_subnet, MYC_subnet	峨参,华鬼臼,臭柏,盾叶鬼臼,小叶莲,鬼臼,窝儿七,山荷叶
P-CRESOL	对甲酚	T	133.3265	FOS_subnet, JUN_subnet, CREB1_subnet, FGF2_subnet, NFKB1_subnet	桑叶,当归,茵陈蒿,独活,没药,川续断
20(R)-GINSENOSIDE RG3	20（r）-人参皂甙rg3	T	130.736	MMP14_subnet, NABA_ECM_REGULATORS, FOS_subnet, HBEGF_subnet, TP53_subnet	西洋参,人参
PROSTRATIN	酪氨酸激酶抑制剂	T	130.3652	CREB1_subnet, CDC42_subnet, RHOA_subnet, RAC1_subnet, MEF2C_subnet	
GAMMA-LINOLENIC ACID	γ-亚麻酸	T	126.9404	GO_COFACTOR_METABOLIC_PROCESS, PTEN_subnet, HRAS_subnet, FOS_subnet, GSE360_L_DONOVANI_VS_M_TUBERCULOSIS_DC_UP	月见草
MONOCROTALINE	单芥子碱	T	119.468	MMP9_subnet, JUN_subnet, AKT1_subnet, KDR_subnet, EGR1_subnet	凹叶野百合,野百合,灯心草,自消容根,自消容,农吉利
ADLUMIDINE	阿鲁替丁	T	117.6568	KDR_subnet, FOS_subnet, YES1_subnet, SRC_subnet, PDGFRB_subnet	升麻,夏天无
BICUCULLINE	双瓜林	T	117.6568	KDR_subnet, FOS_subnet, YES1_subnet, SRC_subnet, PDGFRB_subnet	苦地丁,升麻,延胡索,夏天无
GLYCYRRHIZIC ACID	甘草酸	T	112.524	NFKB1_subnet, GO_COFACTOR_METABOLIC_PROCESS, MMP9_subnet, EGR1_subnet, CREB1_subnet	相思藤,相思子根,甘草头,甘草稍,甘草,甘草节,相思子
GLYCYRRHIZIN	甘草甜素	T	112.524	NFKB1_subnet, GO_COFACTOR_METABOLIC_PROCESS, MMP9_subnet, EGR1_subnet, CREB1_subnet	炙草,甘草头,甘草稍,炙甘草,甘草,甘草节
MONOAMMONIUM	甘草酸单铵盐	T	112.524	NFKB1_subnet, GO_COFACTOR_METABOLIC_PROCES	甘草头,甘草稍,甘草,甘草节

GLYCYRRHIZINATE				S, MMP9_subnet, EGR1_subnet, CREB1_subnet	
ALPHA-LIMONENE	α-柠檬烯	T	112.3219	YES1_subnet, SRC_subnet, ABL1_subnet, KDR_subnet, PTEN_subnet	五味子,干姜,冬凌草,乳香,柴胡,细辛,黄花蒿,茵陈蒿,连翘,大叶香薷,羌活,茴香,橘皮,宽叶羌活,薄荷,苜蓿,海松子,风箱树叶,南鹤虱,生姜,华东蓝刺头,吴茱萸,九里香
D-LIMONENE	d-柠檬烯	T	112.3219	YES1_subnet, SRC_subnet, ABL1_subnet, KDR_subnet, PTEN_subnet	五味子,干姜,橘叶,冬凌草,乳香,枳实,柴胡,枳壳,厚朴,细辛,黄花蒿,茵陈蒿,连翘,荆芥,大叶香薷,羌活,茴香,橘皮,橘白,宽叶羌活,薄荷,橘根,苜蓿,霍香,海松子,南鹤虱,生姜,华东蓝刺头,吴茱萸,九里香,橘络
DIPENTENE	双戊烯	T	112.3219	YES1_subnet, SRC_subnet, ABL1_subnet, KDR_subnet, PTEN_subnet	乳香,大叶香薷,没药,茴香,海松子
L-LIMONENE	L-柠檬烯	T	112.3219	YES1_subnet, SRC_subnet, ABL1_subnet, KDR_subnet, PTEN_subnet	荆芥,紫苏叶,霍香
LIMONEN	柠檬烯	T	112.3219	YES1_subnet, SRC_subnet, ABL1_subnet, KDR_subnet, PTEN_subnet	荆芥
LIMONENE	柠檬油精	T	112.3219	YES1_subnet, SRC_subnet, ABL1_subnet, KDR_subnet, PTEN_subnet	辛夷,麻黄,陈皮,柠檬,当归,小青皮,砂仁,佩兰,缩砂仁,鱼腥草,细辛,青蒿子,花椒,羌活,阿魏,广藿香油,香薷,广藿香叶,败酱草,薄荷,蜀椒,西川芎,川芎,地枫皮,青皮,苏叶,白芷,蔓荆子,青蒿,苦参,广霍香,漏芦,苏梗
HYPERFORIN	贯叶金丝桃素	T	109.3522	MEF2C_subnet, CREB1_subnet, RHOA_subnet, HRAS_subnet, CDC42_subnet	贯叶连翘,地耳草,小连翘
ETHYLBENZENE	乙苯	T	105.5541	EPHA2_subnet, KDR_subnet, PDGFRB_subnet, YES1_subnet, LCK_subnet	苦参
PLASTOQUINONE	质体醌	T	102.8877	TFDP2_subnet, E2F4_subnet, CCND2_subnet, CDK5_subnet, MEF2C_subnet	药用蒲公英
ETHYL ACETATE	乙酸乙酯	T	100.0377	SHH_subnet, TP53_subnet, BAX_subnet, STAT5A_subnet, MCL1_subnet	锁阳,白芷,生姜,矮地茶,吕宋果
PROTOPORPHYRIN	原卟啉	T	97.9721	GO_COFACTOR_METABOLIC_PROCESS, TF_subnet,	罂粟,白屈菜,牛血,延胡索,夏天无,大枣

				GO_SERINE_HYDROLASE_ACTIVITY, MOOTHA_MITOCHONDRIA, GO_ENDOPEPTIDASE_ACTIVITY	
AZELAICACID	壬二酸	T	95.57294	MAPK1_subnet, PTPN1_subnet, PES1_subnet, MAPK3_subnet, HSP90AB1_subnet	党参,木槿皮,当归,黄蒿
TRICHODERMIN	木霉菌素	T	87.55007	EPHA2_subnet, LCK_subnet, PDGFRB_subnet, YES1_subnet, KDR_subnet	
QUERCETIN-3-O-ALPHA-L-RHAMNOPYRANOSIDE	槲皮素-3-邻-α-l-鼠李吡喃糖苷	T	87.24065	CREB1_subnet, MEF2C_subnet, CDC42_subnet, RHOA_subnet, REACTOME_SIGNALING_BY_RECEPTOR_TYROSINE_KINASES	鬼箭锦鸡儿
QUERCETIN-3-O-ALPHA-L-RHAMNOSIDE	槲皮素-3-邻-α-鼠李糖苷	T	87.24065	CREB1_subnet, MEF2C_subnet, CDC42_subnet, RHOA_subnet, REACTOME_SIGNALING_BY_RECEPTOR_TYROSINE_KINASES	白蔹
QUERCETIN-3-RHAMNOSIDE	槲皮素 3-鼠李糖苷	T	87.24065	CREB1_subnet, MEF2C_subnet, CDC42_subnet, RHOA_subnet, REACTOME_SIGNALING_BY_RECEPTOR_TYROSINE_KINASES	
QUERCETRIN	槲皮素	T	87.24065	CREB1_subnet, MEF2C_subnet, CDC42_subnet, RHOA_subnet, REACTOME_SIGNALING_BY_RECEPTOR_TYROSINE_KINASES	侧柏叶
QUERCITRIN	槲皮甙	T	87.24065	CREB1_subnet, MEF2C_subnet, CDC42_subnet, RHOA_subnet, REACTOME_SIGNALING_BY_RECEPTOR_TYROSINE_KINASES	白果叶,油柑叶,贯叶连翘,三白草,红筷子,鱼腥草,合欢花,侧柏叶,虎杖,满山红,金荞麦,虎杖叶,紫金牛,桑寄生,紫花杜鹃,葩蓄,杨梅树皮
DEOXYCORTICOSTERONE	脱氧皮质酮	T	86.48514	AR_subnet, ESR1_subnet, FOS_subnet, NCOR1_subnet, CREB1_subnet	紫河车,熊胆,牛黄
HELENALIN	心菊内酯	T	86.01937	MCL1_subnet, GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, EIF4A1_subnet, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, JUN_subnet	杜仲
MEXICANIN I	墨西哥堆心菊素 I	T	86.01937	MCL1_subnet, GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, EIF4A1_subnet, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, JUN_subnet	
AFZELIN	阿福豆甙	T	82.58068	CREB1_subnet, MEF2C_subnet,	甜地丁,大金牛草,鱼腥草,

				HRAS_subnet, CDC42_subnet, REACTOME_SIGNALING_BY_RECEPTOR_TYROSINE_KINASES	地丁,紫花地丁,木棉花
KAEMPFEROL-3-RHAMNOSIDE	山萘酚 3-鼠李糖苷	T	82.58068	CREB1_subnet, MEF2C_subnet, HRAS_subnet, CDC42_subnet, REACTOME_SIGNALING_BY_RECEPTOR_TYROSINE_KINASES	麻黄,白果叶,油柑叶,大金牛草,鱼腥草
ALPHA,BETA-DIAMINOPROPIONIC ACID	α，β-二氨基丙酸	T	79.05724	RPL5_subnet, TOP2B_subnet, TOP2A_subnet, GMPS_subnet, FBL_subnet	蘑菇
ANISODAMINE	山莨菪碱	T	76.56379	PTPN1_subnet, PES1_subnet, MAPK3_subnet, MAPK1_subnet, JUN_subnet	洋金花,藏茄
GIBBERELLIN A13	赤霉素 a13	T	76.05907	GO_D_METABOLIC_PROCESS, RHOA_subnet, MAPK3_subnet, SRC_subnet, PRKCD_subnet	
NONYLPHENOL	壬基酚	T	75.762	GO_D_METABOLIC_PROCESS, CHIANG_LIVER_CANCER_SUBCLASS_PROLIFERATION_DN, HSIAO_LIVER_SPECIFIC_GENES, AR_subnet, SP1_subnet	五味子
BETA-ALANINE	β-丙氨酸	T	74.94749	GMPS_subnet, TOP2B_subnet, EPHA2_subnet, TOP2A_subnet, PDGFRB_subnet	
BIOPTERIN	生物蝶呤	T	69.28195	GO_COFACTOR_METABOLIC_PROCESS, FOS_subnet, GO_D_METABOLIC_PROCESS, KDR_subnet, NFE2L2.V2	金鱼
FANGCHINOLINE	防己醇灵	T	69.21069	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, GO_HUMORAL_IMMUNE_RESPONSE, NABA_ECM_REGULATORS	虎杖,防己,粉防己,汉防己
MENISIDINE	米尼替丁	T	69.21069	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, GO_HUMORAL_IMMUNE_RESPONSE, NABA_ECM_REGULATORS	防己
THALRUGOSINE	沙丁胺醇	T	69.21069	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES,	银不换,马尾莲

				GO_HUMORAL_IMMUNE_RESPONSE, NABA_ECM_REGULATORS	
PHOSPHOR	磷光体	T	68.64298	TF_subnet, ESR1_subnet, FOS_subnet, GTPBP4_subnet, JUN_subnet	海参,草莓,银耳
OSTHOL	蛇床子素	T	67.15033	GO_D_METABOLIC_PROCESS, HSIAO_LIVER_SPECIFIC_GENES, FGF2_subnet, GO_ENDOPEPTIDASE_ACTIVITY, MYC_subnet	独活,仙鹤草,蛇床子,九里香
OSTHOLE	王草素	T	67.15033	GO_D_METABOLIC_PROCESS, HSIAO_LIVER_SPECIFIC_GENES, FGF2_subnet, GO_ENDOPEPTIDASE_ACTIVITY, MYC_subnet	独活,羌活,大独活,蛇床子
MAYTANSINE	美登素	T	64.00891	CDK5_subnet, HSP90AB1_subnet, ESR1_subnet, PRKN_subnet, AKT1_subnet	
TABERNANTHINE	马山茶碱	T	63.49674	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, GO_HUMORAL_IMMUNE_RESPONSE, NABA_ECM_REGULATORS	
KOLAFLAVANONE	可乐黄酮	T	63.22616	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, GO_HUMORAL_IMMUNE_RESPONSE, NABA_ECM_REGULATORS	臭草
(-)-EPICATECHIN-3-O-GALLATE	(-)-表儿茶素-3-邻没食子酸酯	T	63.21931	ESR1_subnet, MMP9_subnet, STAT3_subnet, FOS_subnet, EGR1_subnet	肉桂
CASSAINE	卡萨因	T	62.83137	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, GO_HUMORAL_IMMUNE_RESPONSE, NABA_ECM_REGULATORS	
CYSTATHIONINE	胱硫醚	T	62.37648	GO_COFACTOR_METABOLIC_PROCESS, TOP2B_subnet, GO_D_METABOLIC_PROCESS, TOP2A_subnet, MOOTHA_MITOCHONDRIA	蘑菇
CATHARANTHI	长春碱	T	60.85569	GO_ADAPTIVE_IMMUNE_RESPONSE_B	长春花

NE				ASED_ON_SOMATIC_RECOMBINATION_OF_IMMUNE_RECEPTORS_BUILT_FROM_IMMUNOGLOBULIN_SUPERFAMILY_DOMAINS, GO_REGULATION_OF_IMMUNE_EFFECTOR_PROCESS, NFKB1_subnet, GO_PRODUCTION_OF_MOLECULAR_MEDIATOR_OF_IMMUNE_RESPONSE, GO_LYMPHOCYTE_MEDIATED_IMMUNITY	
CORILAGIN	鞣云实素	T	60.8434	NABA_ECM_REGULATORS, MAPK3_subnet, KDR_subnet, EPHA2_subnet, MAPK1_subnet	油柑叶,油柑根,蓖麻子,余甘子,地锦草,诃子
ORTHO-AMINOPHENOL	邻氨基苯酚	T	60.52052	CDK5_subnet, HSP90AB1_subnet, SNCA_subnet, ESR1_subnet, YES1_subnet	附子
1-METHYLNAPHTHALENE	1-甲基萘	T	60.36052	GO_D_METABOLIC_PROCESS, TFDP2_subnet, CCND2_subnet, E2F4_subnet, CDK5_subnet	
ISOCITRIC ACID	异柠檬酸	T	56.02993	MOOTHA_MITOCHONDRIA, GO_COFACTOR_METABOLIC_PROCESS, TOP2B_subnet, TOP2A_subnet, TF_subnet	
T-2 TOXIN	t-2 毒素	T	54.97032	KEGG_P53_SIGNALING_PATHWAY, MCL1_subnet, BAX_subnet, SP1_subnet, PRKN_subnet	普洱茶
GALANGIN	高良姜素	T	54.81025	CDK5_subnet, CCND1_subnet, GO_D_METABOLIC_PROCESS, ESR1_subnet, JUN_subnet	大车前,高粱姜,大良姜
CAPRICACID	癸酸	T	53.57109	GO_COFACTOR_METABOLIC_PROCESS, GO_SERINE_HYDROLASE_ACTIVITY, RUAN_RESPONSE_TO_TNF_DN, GO_ENDOPEPTIDASE_ACTIVITY, GO_D_METABOLIC_PROCESS	瓜篓,槟榔,芦荟,鱼腥草,醋柳果,茵陈蒿
DECANOIC ACID	癸酸	T	53.57109	GO_COFACTOR_METABOLIC_PROCESS, GO_SERINE_HYDROLASE_ACTIVITY, RUAN_RESPONSE_TO_TNF_DN, GO_ENDOPEPTIDASE_ACTIVITY, GO_D_METABOLIC_PROCESS	麻黄,当归,喜树,苦参,苏梗
N,N-DIMETHYLTRYPTAMINE	n，n-二甲基色胺	T	51.07311	FOS_subnet, CREB1_subnet, GO_D_METABOLIC_PROCESS, EGR1_subnet, STAT5B_subnet	大蒜,芦竹根
SAQUINAVIR	沙奎那韦	D	50.0978	GO_CYSTEINE_TYPE_ENDOPEPTIDASE	

				_ACTIVITY, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, GO_ENDOPEPTIDASE_ACTIVITY, BAX_subnet, GO_EXTERNAL_SIDE_OF_PLASMA_MEMBRANE	
AGMATINE	胍丁胺	T	49.46719	GO_COFACTOR_METABOLIC_PROCESS, RHOA_subnet, SP1_subnet, PRKCD_subnet, CREB1_subnet	麦角
FERULIC ACID	阿魏酸	T	49.26771	FOS_subnet, GO_COFACTOR_METABOLIC_PROCESS, NFKB1_subnet, ZHOU_INFLAMMATORY_RESPONSE_LPS_UP, MMP9_subnet	伸筋草,升麻,酸枣仁,糯稻根,甘草,木贼,丹参,稻芽,黄连,炙升麻
SODIUM FERULATE	阿魏酸钠	T	49.26771	FOS_subnet, GO_COFACTOR_METABOLIC_PROCESS, NFKB1_subnet, ZHOU_INFLAMMATORY_RESPONSE_LPS_UP, MMP9_subnet	
RESERPINE	利血平	T	47.07226	GO_D_METABOLIC_PROCESS, MODULE_24, ARRB2_subnet, FOS_subnet, CREB1_subnet	萝芙木
JUGLONE	胡桃醌	T	46.63565	GNL3_subnet, MODULE_197, TOP2A_subnet, AR_subnet, MOOTHA_MITOCHONDRIA	核桃仁,胡桃枝,胡桃花,东方核桃,胡桃壳,黑胡桃,化香树果,胡桃油,胡桃根,胡桃叶,胡桃青皮,胡桃树皮,油胡桃,透骨草,胡桃仁,分心木
CROTONICACID	巴豆酸	T	46.61414	GMPS_subnet, HSP90AB1_subnet, RPL5_subnet, AKT1_subnet, TOP2B_subnet	巴豆
3-METHYL-1-BUTANOL	3-甲基-1-丁醇	T	46.24269	TOP2A_subnet, TOP2B_subnet, GO_COFACTOR_METABOLIC_PROCESS, GMPS_subnet, MOOTHA_MITOCHONDRIA	天花粉
ISOAMYL ALCOHOL	异戊醇	T	46.24269	TOP2A_subnet, TOP2B_subnet, GO_COFACTOR_METABOLIC_PROCESS, GMPS_subnet, MOOTHA_MITOCHONDRIA	玫瑰花,山茱萸
PHLORETIN	根皮素	T	45.92688	TOP2A_subnet, JUN_subnet, TOP2B_subnet, MCL1_subnet, MYC_subnet	柠檬叶
LOPINAVIR	洛匹那韦	D	45.22912	GSE3920_UNTREATED_VS_IFNB_TREATED_ENDOTHELIAL_CELL_DN, GTPBP4_subnet, EGR1_subnet, LCK_subnet, PRKCD_subnet	

L-PIPECOLINIC ACID	胡椒碱酸	T	44.47786	MOOTHA_MITOCHONDRIA, BCL6_subnet, GMPS_subnet, MEF2C_subnet, NCOR1_subnet	黑姜,炮姜
PIPECOLICACID	胡椒酸	T	44.47786	MOOTHA_MITOCHONDRIA, BCL6_subnet, GMPS_subnet, MEF2C_subnet, NCOR1_subnet	白饭豆,生姜
O-PYROCATECHUIC ACID	邻焦儿茶酸	T	43.8236	KDR_subnet, PDGFRB_subnet, EPHA2_subnet, YES1_subnet, LCK_subnet	
P-HYDROXYPHENYLPYRUVIC ACID	对羟基苯基丙酮酸	T	42.77425	TOP2A_subnet, MOOTHA_MITOCHONDRIA, GO_COFACTOR_METABOLIC_PROCESS, TOP2B_subnet, TP53_subnet	柠檬根
DEHYDROASCORBICACID	脱氢抗坏血酸	T	42.61323	AKT1_subnet, WALLACE_PROSTATE_CANCER_RACE_UP, MOOTHA_MITOCHONDRIA, MYC_subnet, JUN_subnet	马勃
ANTHRAQUINONE	蒽醌	T	42.37765	GLI1_subnet, GO_CILIARY_PART, AKT1_subnet, EGFR_subnet, SHH_subnet	罗布麻,虎杖
18ALPHA-GLYCYRRHETINIC ACID	18α-甘草次酸	T	41.11892	GO_D_METABOLIC_PROCESS, MOOTHA_MITOCHONDRIA, GO_COFACTOR_METABOLIC_PROCESS, MMP9_subnet, NFKB1_subnet	炙草,甘草头,甘草稍,炙甘草,甘草,甘草节
18BETA-GLYCYRRHETINIC ACID	18β-甘草次酸	T	41.11892	GO_D_METABOLIC_PROCESS, MOOTHA_MITOCHONDRIA, GO_COFACTOR_METABOLIC_PROCESS, MMP9_subnet, NFKB1_subnet	炙草,甘草头,甘草稍,炙甘草,甘草,甘草节
GLYCYRRHETINIC ACID	甘草次酸	T	41.11892	GO_D_METABOLIC_PROCESS, MOOTHA_MITOCHONDRIA, GO_COFACTOR_METABOLIC_PROCESS, MMP9_subnet, NFKB1_subnet	炙草,甘草头,甘草稍,炙甘草,甘草,甘草节
3,3',5'-TRIIODOTHYRONINE	3,3'，5'-三碘甲状腺素	T	41.0899	ESR2_subnet, BAX_subnet, TF_subnet, FOS_subnet, AR_subnet	
ALPHA-PINENE	α--烯	T	40.97237	GO_SERINE_HYDROLASE_ACTIVITY, GO_D_METABOLIC_PROCESS, GO_ENDOPEPTIDASE_ACTIVITY, MODULE_24, MOOTHA_MITOCHONDRIA	党参,辛荑,麻黄,陈皮,狼毒,当归,松节,马兜铃,砂仁,佩兰,缩砂仁,鱼腥草,细辛,花椒,羌活,阿魏,香薷,败酱草,薄荷,樟脑,千年健,蜀椒,西川芎,川芎,地枫皮,艾叶,吴芋,西党,苏叶,海风藤,白芷,蔓荆子,甘松,菊花,苦参
MIMOSINE	含羞草素	T	40.91006	TP53_subnet, FBL_subnet, CTNNB1_subnet, SMAD2_subnet,	密蒙花

				MYC_subnet	
D-GLYCERIC ACID	d-甘油酸	T	38.31781	TOP2B_subnet, TOP2A_subnet, GO_COFACTOR_METABOLIC_PROCESS, GMPS_subnet, GO_D_METABOLIC_PROCESS	黑大豆
UREA	尿素	T	37.99421	NFATC2_subnet, FOS_subnet, MOOTHA_MITOCHONDRIA, GO_COFACTOR_METABOLIC_PROCESS, MYOD1_subnet	黄甘草,夜明砂,人中白,牛血,马勃,五灵脂,甘草
METHYL MERCAPTAN	甲硫醇	T	37.26482	HSP90AB1_subnet, RPL5_subnet, GMPS_subnet, TOP2B_subnet, TOP2A_subnet	莱菔,枇杷叶,莱菔子
CINNAMICACID	肉桂酸	T	37.10548	GO_SERINE_HYDROLASE_ACTIVITY, GO_ENDOPEPTIDASE_ACTIVITY, SNAI1_subnet, ESR1_subnet, MAPK3_subnet	桂皮,桂枝,大车前,茴香,玄参,安息香,苏合香,枸杞子,谷壳,肉桂
TRANS-CINNAMIC ACID	反肉桂酸	T	37.10548	GO_SERINE_HYDROLASE_ACTIVITY, GO_ENDOPEPTIDASE_ACTIVITY, SNAI1_subnet, ESR1_subnet, MAPK3_subnet	樟树子,桂丁,肉桂叶,桂枝,制桂枝,茴香根茎叶,香樟根,樟脑,樟树叶,樟木,枸杞子,肉桂,樟树皮
CIS-GERANIOL	顺式香叶醇	T	36.97602	GO_COFACTOR_METABOLIC_PROCESS, HSP90AB1_subnet, CDK5_subnet, ESR1_subnet, MYC_subnet	陈皮
GERANIOL	香叶醇	T	36.97602	GO_COFACTOR_METABOLIC_PROCESS, HSP90AB1_subnet, CDK5_subnet, ESR1_subnet, MYC_subnet	五味子,大芭蕉,老鹳草,辛荑,干姜,麻黄,大蒜,千金花,金银花,短柱八角,玫瑰花,九里香根,白玉兰,柴胡,佩兰,花椒,半边苏,胡荽,啤酒花,蜀椒,青蒜,忍冬藤,双花,地枫皮,白兰花,芸香草,谷壳,苦参实,生姜,苦参,九里香
NEROL	神经醇	T	36.97602	GO_COFACTOR_METABOLIC_PROCESS, HSP90AB1_subnet, CDK5_subnet, ESR1_subnet, MYC_subnet	辛荑,陈皮,金银花,玫瑰花,肝风草,砂仁,佩兰,缩砂仁,细辛,橘皮,双花,苏叶,生姜,苏梗
CARFILZOMIB	卡非佐米	D	36.26945	RASSF1_subnet, TP53_subnet, HSP90AB1_subnet, NFKB1_subnet, CCND1_subnet	
METHYL PHENYL CARBINOL	甲基苯基甲醇	T	35.63056	GO_D_METABOLIC_PROCESS, HSIAO_LIVER_SPECIFIC_GENES, GO_COFACTOR_METABOLIC_PROCESS, GTPBP4_subnet, TOP2B_subnet	茶叶,川芎
N-HEXYL-BETA-	正己基	T	35.2088	MOOTHA_MITOCHONDRIA,	党参,麦角

D-GLUCOPYRANOSIDE	β-d-吡喃葡萄糖苷			EGR1_subnet, AR_subnet, ESR1_subnet, JUN_subnet	
MAGNESIUM CARBONATE	碳酸镁	T	34.1554	CDK5_subnet, BMP4_subnet, MYC_subnet, MYOD1_subnet, SHH_subnet	蛤壳
TROPOLONE	托酚酮	T	33.8332	PRKN_subnet, SNCA_subnet, GO_D_METABOLIC_PROCESS, RAC1_subnet, CDC42_subnet	
VITAMIN B12	维生素 b12	T	33.22757	SHH_subnet, SMAD2_subnet, FGF2_subnet, BMP4_subnet, SMAD4_subnet	黑大豆,当归,人参,醋柳果,紫苏,冬虫夏草,枸杞子,大枣
N-PROPANOL	正丙醇	T	33.02975	TOP2B_subnet, TOP2A_subnet, SRC_subnet, EGR1_subnet, CDK5_subnet	生姜
POLYSORBATE-80	聚山梨酯 80	T	32.83031	TOP2B_subnet, TOP2A_subnet, PIK3R3_subnet, PES1_subnet, GMPS_subnet	
OXALICACID	草酸	T	32.27949	GO_COFACTOR_METABOLIC_PROCESS, TOP2A_subnet, TOP2B_subnet, MOOTHA_MITOCHONDRIA, CREB1_subnet	山楂,百部,醋柳果,黄蒿,菠菜,异株荨麻
O-CRESOL	邻甲酚	T	32.22728	GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, GO_ENDOPEPTIDASE_ACTIVITY, ERBB3_subnet, GO_ANATOMICAL_STRUCTURE_HOMEOSTASIS	当归,乳香,茵陈蒿,西川芎,川芎
VENOTERPINE	喜树次碱	T	32.01071	CDK5_subnet, HSP90AB1_subnet, ESR1_subnet, GMPS_subnet, AKT1_subnet	喜树,川续断
PINOCEMBRIN	松属素	T	30.4631	NABA_ECM_REGULATORS, MAPK3_subnet, MAPK1_subnet, FGF2_subnet, JUN_subnet	光果甘草,胡椒
ECDYSONE	蜕皮激素	T	30.27975	GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, NABA_ECM_REGULATORS, GO_ENDOPEPTIDASE_ACTIVITY, NCOR1_subnet	贯众,白僵蚕,小叶贯众
PHENYLPYRUVIC ACID	苯丙酮酸	T	28.86522	GO_COFACTOR_METABOLIC_PROCESS, MOOTHA_MITOCHONDRIA, MODULE_24, TOP2B_subnet, NFE2L2.V2	安息香
RYANODINE	雷诺丁	T	28.52202	GO_SERINE_HYDROLASE_ACTIVITY, GO_ENDOPEPTIDASE_ACTIVITY, GO_ANATOMICAL_STRUCTURE_HOMEOSTASIS, CREB1_subnet, SRC_subnet	

NEREISTOXIN	沙蚕毒素	T	27.91496	TF_subnet, GO_ANATOMICAL_STRUCTURE_HOMEOSTASIS, FOS_subnet, GRB2_subnet, SRC_subnet	干姜,橘皮,生姜
OCTOPAMINE	章鱼胺	T	27.49963	GO_SERINE_HYDROLASE_ACTIVITY, GO_ENDOPEPTIDASE_ACTIVITY, MODULE_24, FOS_subnet, STAT3_subnet	辣椒头,辣椒,辣椒茎
PYRIMIDINONE	嘧啶酮	T	27.44128	GO_COFACTOR_METABOLIC_PROCESS, GMPS_subnet, KRAS_subnet, NRAS_subnet, TOP2B_subnet	蘑菇,玉蜀黍,八角茴香,甘蔗,牛乳,蜂蜜
22,23-DIHYDROSTIGMASTEROL	22,23-二氢豆甾醇	T	26.6386	SP1_subnet, ESR1_subnet, NCOR1_subnet, CREB1_subnet, TP53_subnet	木香
BETA-DIHYDROFUCOSTEROL	β-二氢岩藻甾醇	T	26.6386	SP1_subnet, ESR1_subnet, NCOR1_subnet, CREB1_subnet, TP53_subnet	
BETA-SITOSTEROL	β-谷固醇	T	26.6386	SP1_subnet, ESR1_subnet, NCOR1_subnet, CREB1_subnet, TP53_subnet	阴行草,孩儿参,赤芍,雪上一枝蒿,南沙参,茵陈,板蓝根,白附子,白芍,炙黄芪,败酱草,香掾,穿心莲,关木通,刘寄奴,黄芪,海风藤,蔓荆子,大青叶,川木通,红芪,黄柏
GAMMA-SITOSTEROL	γ-谷固醇	T	26.6386	SP1_subnet, ESR1_subnet, NCOR1_subnet, CREB1_subnet, TP53_subnet	清风藤,黄甘草,蟾酥,肉苁蓉,木槿皮,黑大豆,木通,广防己,三七,红花,金银花,蒲黄,板蓝根,天南星,人参,桂枝,巴豆,骨碎补,黄花蒿,醋柳果,羌活,车前,大车前,仙鹤草,木香,橘皮,半夏,霍香,川芎,葛根,冬虫夏草,何首乌,杜仲,黄芩,天麻,甘草,川续断,黄芪,小麦,白果,丹参,枸杞子,蔓荆子,五加皮,华东蓝刺头,石苇,防风,大青叶,小叶贯众,黄柏,刺五加
SITOSTEROL	谷甾醇	T	26.6386	SP1_subnet, ESR1_subnet, NCOR1_subnet, CREB1_subnet, TP53_subnet	洋地黄叶,鹅不食草,大活血,寒食,皂荚,水杨梅,猪牙皂,紫贝齿,香掾,牙皂,黑木耳,石南藤,大血藤
HOMOSERINE	高丝氨酸	T	26.23355	TOP2B_subnet, TOP2A_subnet, HSP90AB1_subnet, MOOTHA_MITOCHONDRIA, TP53_subnet	黄精
L-HOMOSERINE	左旋高丝	T	26.23355	TOP2B_subnet, TOP2A_subnet,	紫檀,按叶,刀豆

	氨酸			HSP90AB1_subnet, MOOTHA_MITOCHONDRIA, TP53_subnet	
HYDROCINNAMIC ACID	氢肉桂酸	T	26.15287	MOOTHA_MITOCHONDRIA, GO_COFACTOR_METABOLIC_PROCESS, CDK5_subnet, TOP2A_subnet, TOP2B_subnet	槲寄生
ALLANTOIC ACID	尿囊酸	T	26.08547	GO_COFACTOR_METABOLIC_PROCESS, GMPS_subnet, TOP2B_subnet, TOP2A_subnet, JUN_subnet	紫藤
2-ETHYL-HEXANOL	2-乙基己醇	T	25.5606	GSE13485_PRE_VS_POST_YF17D_VACCINATION_PBMC_DN, RAC1_subnet, CDC42_subnet, RHOA_subnet, MAPK1_subnet	锁阳
LAWSONE	散沫花素	T	25.45299	GO_D_METABOLIC_PROCESS, ABL1_subnet, YES1_subnet, SRC_subnet, GO_ENDOPEPTIDASE_ACTIVITY	荜拔,无叶藤,急性子
LAWSONIN	硬柱石	T	25.45299	GO_D_METABOLIC_PROCESS, ABL1_subnet, YES1_subnet, SRC_subnet, GO_ENDOPEPTIDASE_ACTIVITY	
MUCICACID	粘酸	T	25.3302	GO_COFACTOR_METABOLIC_PROCESS, GO_D_METABOLIC_PROCESS, FOS_subnet, MMP9_subnet, TOP2B_subnet	
CHOLEST-4-ENE-3-ONE	胆甾-4-烯-3-一	T	25.24435	GO_D_METABOLIC_PROCESS, HSIAO_LIVER_SPECIFIC_GENES, MOOTHA_MITOCHONDRIA, GO_ENDOPEPTIDASE_ACTIVITY, STAT3_subnet	麝香,相思子
1,4-NAPHTHOQUINONE	1,4-萘醌	T	25.03195	YES1_subnet, MOOTHA_MITOCHONDRIA, ABL1_subnet, GO_COFACTOR_METABOLIC_PROCESS, SRC_subnet	胡桃仁
CARNOSINE	肌肽	T	24.97666	HSP90AB1_subnet, GMPS_subnet, TOP2B_subnet, TOP2A_subnet, AKT1_subnet	蘑菇,蛤蚧,鳗鲡鱼
DIGITOXIN	洋地黄毒	T	24.07224	GO_COFACTOR_METABOLIC_PROCESS, MAPK3_subnet, MMP9_subnet, MAPK1_subnet, SRC_subnet	
STACHYDRINE	水苏碱	T	23.91316	TOP2B_subnet, TOP2A_subnet, HSP90AB1_subnet, GO_ENDOPEPTIDASE_ACTIVITY, STAT3_subnet	苜蓿,益母草,菊花
PYRIDOXINE	吡哆醇	T	23.87751	GO_COFACTOR_METABOLIC_PROCES	除虫菊,蘑菇,玉蜀黍,甘蔗,

				S, TOP2B_subnet, TOP2A_subnet, NFE2L2.V2, MODULE_24	牛乳,蜂蜜
VITAMIN B6	维生素 b6	T	23.87751	GO_COFACTOR_METABOLIC_PROCESS, TOP2B_subnet, TOP2A_subnet, NFE2L2.V2, MODULE_24	蘑菇,八角茴香,甘蔗,牛乳,蜂蜜
2-FURALDEHYDE	2-呋喃醛	T	23.33908	GSE13485_PRE_VS_POST_YF17D_VACCINATION_PBMC_DN, GO_COFACTOR_METABOLIC_PROCESS, NFE2L2.V2, PTEN_subnet, TP53_subnet	泽泻,金银花,锁阳,紫菜,红车轴草,茵陈蒿,苍术,黄蒿,双花,山茱萸
2-FURANCARBOXALDEHYDE	2-呋喃甲醛	T	23.33908	GSE13485_PRE_VS_POST_YF17D_VACCINATION_PBMC_DN, GO_COFACTOR_METABOLIC_PROCESS, NFE2L2.V2, PTEN_subnet, TP53_subnet	天花粉
FURALDEHYDE	糠醛	T	23.33908	GSE13485_PRE_VS_POST_YF17D_VACCINATION_PBMC_DN, GO_COFACTOR_METABOLIC_PROCESS, NFE2L2.V2, PTEN_subnet, TP53_subnet	茵陈
OROTICACID	乳清酸	T	23.15596	TOP2B_subnet, TOP2A_subnet, GMPS_subnet, TP53_subnet, GO_ENDOPEPTIDASE_ACTIVITY	牛乳
SE-METHYL-L-SELENOCYSTEINE	甲基-1-硒代半胱氨酸	T	22.48677	GO_COFACTOR_METABOLIC_PROCESS, KRAS_subnet, NRAS_subnet, TP53_subnet, HRAS_subnet	人参
VITAMIN B5	维生素 b5	T	22.41873	GO_COFACTOR_METABOLIC_PROCESS, GMPS_subnet, JUN_subnet, CTNNB1_subnet, TP53_subnet	人参,白果,枸杞子,大枣
1-O-OCTADECANOYL GLYCEROL	1-o-十八碳烯基甘油	T	22.22378	TOP2B_subnet, TOP2A_subnet, GMPS_subnet, JUN_subnet, GO_ENDOPEPTIDASE_ACTIVITY	

注：“类型”栏标注"D"表示该化合物为初始输入药物，"T"表示天然产物（中药）成分。

附表 3. 抗冠状病毒活性天然产物成分

Natural product composition	天然产物成分	引用次数	引用总计	Tcm-1	Tcm-2	参考文献
Glycyrrhizin	甘草酸	435	435	None	Glycyrrhizin	Cinatl et al. 2003
GinsenosideRb1	人参皂甙 Rb1	199	199	None	GinsenosideRb1	Wu et al. 2004
Reserpine	利血平	199	199	None	Reserpine	Wu et al. 2004
Aescin	七叶皂甙	199	199	None	None	Wu et al. 2004
Aloe Emodin	芦荟大黄素	113	113	None	None	Lin et al. 2005
Hesperetin	橙皮素	113	113	None	None	Lin et al. 2005
Emodin	大黄素	72		Emodin	None	Ho et al. 2007
Emodin	大黄素	34	111	Emodin	None	Schwarz et al. 2011
Emodin	大黄素	5		Emodin	None	Schwarz et al. 2011
Tetra-O-Galloyl-B-D-Glucose (Tgg)	四 -O- 没 食 子 酰 -β-d-葡萄糖（TGG）	81	81	None	None	Yi et al. 2004

Luteolin	木犀草素	81	81	None	None	Yi et al. 2004
Quercetin	槲皮素	42	61	None	None	Chiow et al. 2016
Quercetin	槲皮素	19		None	None	Nguyen et al. 2012
Tannic Acid	单宁酸	61	61	None	None	Chen et al. 2005
3-Isotheaflavin-3-Gallate (Tf2B)	3-异黄素-3-没食子酸酯（TF2B）	61	61	None	None	Chen et al. 2005
Theaflavin-3,3'-Digallate (Tf3)	茶黄素 3,3'-对苯二甲酸（TF3）	61	61	None	None	Chen et al. 2005
Roem	香椿铃	48	48	None	None	Chen et al. 2008
Curcumin	姜黄素	44	44	None	None	Wen et al. 2007
Ferruginol	弥罗松酚	44	44	None	None	Wen et al. 2007
Dehydroabieta-7-One	脱氢枞醇	44	44	None	None	Wen et al. 2007
Sugiol	柳杉酚	44	44	None	None	Wen et al. 2007
Cryptojaponol	柳杉树脂酚	44	44	None	None	Wen et al. 2007
[8B-Hydroxyabieta-9(11),13-Dien-12-One)]	[8β-羟基松香-9（11）,13-二亚乙基三胺-12-一）]	44	44	None	None	Wen et al. 2007
7B-Hydroxydeoxycryptojaponol	7β-羟基脱氧隐皂甙	44	44	None	None	Wen et al. 2007
6,7-Dehydroroyleanone	6,7-脱氢基丙酮	44	44	None	None	Wen et al. 2007
3B,12-Diacetoxyabieta-6,8,11,13-Tetraene	3β,12-二乙酰氧基松香-6,8,11,13-四烯	44	44	None	None	Wen et al. 2007
Pinusolidic Acid	松柏酸	44	44	None	None	Wen et al. 2007
Forskolin	毛喉萜	44	44	None	None	Wen et al. 2007
Cedrane-3B,12-Diol	香松烷-3β,12-二醇	44	44	None	None	Wen et al. 2007
A-Cadinol	α-杜松醇	44	44	None	None	Wen et al. 2007
Betulinic Acid	桦木酸	44	44	None	Betulinic Acid	Wen et al. 2007
Betulonic Acid	桦木酮酸	44	44	None	None	Wen et al. 2007
Hinokinin	扁白脂素	44	44	None	None	Wen et al. 2007
Savinin	桧脂素	44	44	None	None	Wen et al. 2007
4,4'-O-Benzoylisolariciresinol	4,4'-O-苯甲酰基异拉西里醇	44	44	None	None	Wen et al. 2007
Honokiol	和厚朴酚	44	44	Honokiol	None	Wen et al. 2007
Magnolol	厚朴酚	44	44	Magnolol	None	Wen et al. 2007
Niclosamide	氯硝柳胺	44	44	None	None	Wen et al. 2007
Valinomycin	缬氨霉素	44	44	None	None	Wen et al. 2007
Quercitrin	槲皮苷	42	42	None	Quercitrin	Chiow et al. 2016
Pentoxifylline	己酮可可碱	42	42	None	None	Martín et al. 2013
Myricetin	杨梅素	36	36	Myricetin	Myricetin	Yu et al. 2012
Scutellarein	野黄芩素	36	36	None	None	Yu et al. 2012
Saikosaponin B2	柴胡皂苷 B2	27	27	None	None	Cheng et al. 2006
Gallocatechin Gallate (Gcg)	没食子儿茶素没食子酸酯（GCG）	19	22	None	None	Nguyen et al. 2012
Gallocatechin Gallate (Gcg)	没食子儿茶素没食子酸酯（GCG）	3		None	None	Roh et al. 2012
Hirsutenone	(4E)-1,7-双(3,4-二羟基苯基)-4-庚烯-3-酮	19	19	None	None	Park et al. 2012
Epigallocatechin Gallate	表没食子儿茶素没食子酸酯	19	19	None	None	Nguyenet al. 2012
Juglanin	胡桃宁	16	16	None	None	Schwarz et al. 2014
Papyriflavonol A	泛醇黄酮 A	15	15	None	None	Park et al. 2017
Chalcones	查耳酮	10	10	None	None	Park et al. 2017

Resveratrol	白藜芦醇	9	9	None	None	Lin et al. 2017
Kaempferole	山奈酚	5	5	None	None	Schwarz et al. 2012
Kaempferole Glycosides	山奈酚苷	5	5	None	None	Schwarz et al. 2012
Catechin Gallate	儿茶素没食子酸酯	3	3	None	None	Roh et al. 2012
Herbacetin	草质素	0	0	None	None	Jo et al. 2019
Isobavachalcone	异补骨脂查耳酮	0	0	None	None	Jo et al. 2019
Quercetin 3-B-D-Glucoside	槲皮素 3-β-d-葡萄糖苷	0	0	None	None	Jo et al. 2019
Helichrysetin	蜡菊亭	0	0	None	None	Jo et al. 2019

附表 4. COVID-19 药物与候选芳香化合物及其分子机制

Compound name	**名称**	**类型**	**相关性**	**显著关联基因模块（Top5）**
4,5-DIMETHYLTHIAZOLE	4,5-二甲基噻唑	A	1244.519	STAT3_subnet, TP53_subnet, NFKB1_subnet, AKT1_subnet, STAT5A_subnet
WORTMANNIN	渥曼青霉素	A	1047.178	TP53_subnet, NFKB1_subnet, AKT1_subnet, FOS_subnet, ESR1_subnet
RITONAVIR	利托那韦	D	708.9371	STAT3_subnet, TP53_subnet, NFKB1_subnet, AKT1_subnet, STAT5A_subnet
BENZENE	苯	A	558.8391	MCL1_subnet, BAX_subnet, TP53_subnet, ESR1_subnet, PTEN_subnet
DIHYDROCUMINIC ALCOHOL	二氢枯黄醇	A	485.9092	WWOX_subnet, SNAI1_subnet, LCK_subnet, NRAS_subnet, NFKB1_subnet
DIHYDROCUMINYL ALCOHOL	二氢枯烯醇	A	485.9092	WWOX_subnet, SNAI1_subnet, LCK_subnet, NRAS_subnet, NFKB1_subnet
L-ALANYL-L-GLUTAMINE	l-丙氨酰-l-谷氨酰胺	A	482.8761	CREB1_subnet, CDH1_subnet, STAT5B_subnet, CDC42_subnet, KDR_subnet
NELFINAVIR	奈非那韦	D	478.8154	GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, TP53_subnet, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, AR_subnet, AKT1_subnet
CHLOROQUINE	氯喹	D	443.9332	AKT1_subnet, NFKB1_subnet, SRC_subnet, MMP9_subnet, TP53_subnet
DIBUTYL PHTHALATE	邻苯二甲酸二丁酯	A	426.8389	PTPN1_subnet, NFKB1_subnet, AR_subnet, MAPK1_subnet, SP1_subnet
PRASTERONE	普拉雄酮	A	423.9931	AR_subnet, CREB1_subnet, EGR1_subnet, FOS_subnet, GO_DRUG_METABOLIC_PROCESS
DIALLYL TRISULFIDE	二硫化三烯丙基	A	420.3887	NFKB1_subnet, FOS_subnet, EGFR_subnet, PRKN_subnet, TP53_subnet
ACETIC ALDEHYDE	乙醛	A	411.9857	CREB1_subnet, SP1_subnet, MMP9_subnet, STAT3_subnet, AR_subnet
2,2-BICHAVICOL	2,2-二甲酚	A	395.2682	MMP9_subnet, FGF2_subnet, NFKB1_subnet, AR_subnet, JUN_subnet
(E)-ANETHOLE	（e）-茴香烯	A	391.7848	NFKB1_subnet, SNAI1_subnet, PTEN_subnet, KEGG_CHRONIC_MYELOID_LEUKEMIA,

				STAT3_subnet
TRANS-ANETHOLE	反式茴香烯	A	391.7848	NFKB1_subnet, SNAI1_subnet, PTEN_subnet, KEGG_CHRONIC_MYELOID_LEUKEMIA, STAT3_subnet
DIALLYL DISULFUDE	二烯丙基二硫	A	381.3935	GO_SERINE_HYDROLASE_ACTIVITY, GO_ENDOPEPTIDASE_ACTIVITY, MYC_subnet, CDK5_subnet, NFATC1_subnet
RIBAVIRIN	利巴韦林	D	376.0455	LCK_subnet, STAT3_subnet, NFKB1_subnet, STAT5A_subnet, EGR1_subnet
CINNAMALDEHYDE	肉桂醛	A	372.6276	FOS_subnet, JUN_subnet, PTPN1_subnet, NFKB1_subnet, MMP9_subnet
L-ARGININE	精氨酸	A	316.5091	EGFR_subnet, SRC_subnet, TGM2_subnet, FOS_subnet, KDR_subnet
ARGEOL	粗酒石	A	316.5091	EGFR_subnet, SRC_subnet, TGM2_subnet, FOS_subnet, KDR_subnet
OCTADECANOIC ACID	十八烷酸	A	306.9626	ESR1_subnet, ESR2_subnet, NCOR1_subnet, AR_subnet, SRC_subnet
2,3-BENZOPYRROLE	2,3-苯并吡咯	A	284.1591	FOS_subnet, MMP9_subnet, EGR1_subnet, ESR1_subnet, CREB1_subnet
INDOLE	吲哚	A	284.1591	FOS_subnet, MMP9_subnet, EGR1_subnet, ESR1_subnet, CREB1_subnet
PHENYL ETHYL ALCOHOL	苯乙醇	A	275.4931	GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, GO_ENDOPEPTIDASE_ACTIVITY, BAX_subnet, BMS1_subnet
BENZYL ISOTHIOCYANATE	异硫氰酸苄酯	A	251.6309	ESR2_subnet, MYC_subnet, EGFR_subnet, NFKB1_subnet, MMP9_subnet
DIBUNOL	地丁酚	A	251.1722	GO_DRUG_METABOLIC_PROCESS, GO_COFACTOR_METABOLIC_PROCESS, SRC_subnet, HSIAO_LIVER_SPECIFIC_GENES, ESR1_subnet
ACETOVANILLONE	乙酰香草醛	A	249.7875	SRC_subnet, MMP9_subnet, RHOA_subnet, AKT1_subnet, RAC1_subnet
ETHYLENIMINE	乙炔亚胺	A	249.2398	CDK5_subnet, TF_subnet, GTPBP4_subnet, MMP9_subnet, CDC42_subnet
MYCOPHENOLATE MOFETIL	霉酚酸酯	D	238.0351	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, GO_HUMORAL_IMMUNE_RESPONSE, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, REACTOME_COMPLEMENT_CASCADE
INDINAVIR	茚地那韦	D	233.0818	GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY,

				GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY,
LIMONENE	柠檬烯	A	225.9022	STAT5B_subnet, STAT3_subnet, AKT1_subnet YES1_subnet, SRC_subnet, ABL1_subnet, KDR_subnet, PTEN_subnet
BUTYL 4-HYDROXYBENZOATE	4-羟基苯甲酸丁酯	A	224.8339	STAT5A_subnet, AR_subnet, STAT5B_subnet, FOS_subnet, NCOR1_subnet
P-CRESOL	对甲酚	A	223.6172	FOS_subnet, JUN_subnet, CREB1_subnet, FGF2_subnet, NFKB1_subnet
OCTADECANE	十八烷	A	206.2233	PRKN_subnet, GRK3_subnet, OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet
ALPHA-LINOLNIC ACID	α-亚麻酸	A	205.2858	NCOR1_subnet, ESR2_subnet, ESR1_subnet, RUAN_RESPONSE_TO_TNF_DN, SP1_subnet
CEVADIC ACID	头孢酸	A	200.864	OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet, OR4S2_subnet, OR51B4_subnet
TIGLIC ACID	提香酸	A	200.864	OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet, OR4S2_subnet, OR51B4_subnet
AMYL FURAN-2-CARBOXYLATE	呋喃-2-羧酸戊酯	A	200.2531	OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet, OR4S2_subnet, OR51B4_subnet
AMYL SULFHYDRATE	戊基水合物	A	200.2531	OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet, OR4S2_subnet, OR51B4_subnet
LINOLEIC	亚油酸	A	193.2053	NCOR1_subnet, CREB1_subnet, SP1_subnet, HSIAO_LIVER_SPECIFIC_GENES, MAPK1_subnet
METHYL SALICYCLATE	水杨酸甲酯	A	187.937	JUN_subnet, ERBB3_subnet, FOS_subnet, EGR1_subnet, PTPN1_subnet
ISOEUGENOL	异丁香酚	A	186.9832	GO_COFACTOR_METABOLIC_PROCESS, GO_DRUG_METABOLIC_PROCESS, OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet
CYCLAMAL	环磺酸盐	A	185.26	OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet, OR4S2_subnet, OR51B4_subnet
BUTYRIC ACID, PHENYL ESTER	丁酸，苯酯	A	181.9789	HSP90AB1_subnet, JUN_subnet, NFKB1_subnet, AR_subnet, CREB1_subnet
BENZYL CARBINYL ACETATE	乙酸苄酯	A	181.9789	HSP90AB1_subnet, JUN_subnet, NFKB1_subnet, AR_subnet, CREB1_subnet
QUINOLINE	喹啉	A	176.336	EGFR_subnet, CTNNB1_subnet, JUN_subnet, MYC_subnet, RHOA_subnet
UNDECANAL	十一醛	A	173.6282	GNAL_subnet, OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet, OR4S2_subnet
BENZOPYRIDINE	苯并吡啶	A	172.7912	MDK_subnet, EGFR_subnet, HSP90AB1_subnet, MYC_subnet, CTNNB1_subnet
BUTYRIC ACID	丁酸	A	169.1115	FOS_subnet, GNGT1_subnet, ARRB2_subnet, GNAL_subnet, RHOA_subnet
SALICYLIC ACID	水杨酸	A	167.2147	STAT3_subnet, NFKB1_subnet, ANGPT2_subnet, MMP9_subnet,

(E)-METHYL ISOEUGENOL	（e）-甲基异丁香酚	A	163.2316	GO_DRUG_METABOLIC_PROCESS OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet, OR4S2_subnet, OR51B4_subnet
DIALLYL SULFIDE	二烯丙基硫	A	159.2772	GO_CYSTEINE_TYPE_ENDOPEPTIDASE_ACTIVITY, RASSF1_subnet, GO_CYSTEINE_TYPE_PEPTIDASE_ACTIVITY, TP53_subnet, MMP9_subnet
3-METHYLTHIOPROPYLAMINE	3-甲硫基丙胺	A	155.9626	CCND1_subnet, GO_IMMUNE_RESPONSE_REGULATING_CELL_SURFACE_RECEPTOR_SIGNALING_PATHWAY, GMPS_subnet, GO_ENDOPEPTIDASE_ACTIVITY, RPL5_subnet
1-EICOSANOL	1-二十烷醇	A	150.3026	LCK_subnet, ABL1_subnet, KDR_subnet, EPHA2_subnet, PDGFRB_subnet
ECOSANOL	生态醇	A	150.3026	LCK_subnet, ABL1_subnet, KDR_subnet, EPHA2_subnet, PDGFRB_subnet
EICOSAN-1-OL	二十烷醇	A	150.3026	LCK_subnet, ABL1_subnet, KDR_subnet, EPHA2_subnet, PDGFRB_subnet
EICOSANOL	二十烷醇	A	150.3026	LCK_subnet, ABL1_subnet, KDR_subnet, EPHA2_subnet, PDGFRB_subnet
1-AMINOHEXANE	1-氨基己烷	A	149.6079	CCND1_subnet, GO_IMMUNE_RESPONSE_REGULATING_CELL_SURFACE_RECEPTOR_SIGNALING_PATHWAY, GO_ENDOPEPTIDASE_ACTIVITY, PRKN_subnet, HSP90AB1_subnet
SQUALENE	角鲨烯	A	145.6421	LCK_subnet, JUN_subnet, NFKB1_subnet, MMP9_subnet, SRC_subnet
CORIANDROL	芫荽醇	A	145.0551	MMP14_subnet, GO_COFACTOR_METABOLIC_PROCESS, HBEGF_subnet, GO_DRUG_METABOLIC_PROCESS, TGM2_subnet
LINALOOL	芳樟醇	A	145.0551	MMP14_subnet, GO_COFACTOR_METABOLIC_PROCESS, HBEGF_subnet, GO_DRUG_METABOLIC_PROCESS, TGM2_subnet
AMINOHYDROCINNAMIC ACID	氨基肉桂酸	A	144.3527	CCND1_subnet, GO_IMMUNE_RESPONSE_REGULATING_CELL_SURFACE_RECEPTOR_SIGNALING_PATHWAY, GMPS_subnet, GO_ENDOPEPTIDASE_ACTIVITY, PRKN_subnet
IODOQUINOL	碘喹醇	A	143.7128	MDK_subnet, GNGT1_subnet, ARRB2_subnet, MCL1_subnet, PTPN1_subnet

3-METHYLBUTYRIC ACID	3-甲基丁酸	A	142.8269	GO_COFACTOR_METABOLIC_PROCESS, MOOTHA_MITOCHONDRIA, TOP2B_subnet, GSE1925_3H_VS_24H_IFNG_STIM_MACROPHAGE_UP, TOP2A_subnet
ISOVALERIC ACID	异戊酸	A	142.8269	GO_COFACTOR_METABOLIC_PROCESS, MOOTHA_MITOCHONDRIA, TOP2B_subnet, GSE1925_3H_VS_24H_IFNG_STIM_MACROPHAGE_UP, TOP2A_subnet
ALPHA-AMINOISOVALERIC ACID	α-氨基异戊酸	A	142.7059	CCND1_subnet, GO_IMMUNE_RESPONSE_REGULATING_CELL_SURFACE_RECEPTOR_SIGNALING_PATHWAY, GO_ENDOPEPTIDASE_ACTIVITY, GMPS_subnet, HSP90AB1_subnet
2-BIPHENYLOL	2-联苯酚	A	141.8333	LCK_subnet, PDGFRB_subnet, ABL1_subnet, YES1_subnet, KDR_subnet
HEXADECANOIC ACID	十六烷酸	A	136.5528	HSIAO_LIVER_SPECIFIC_GENES, GO_COFACTOR_METABOLIC_PROCESS, MMP9_subnet, AKT1_subnet, FOS_subnet
PALMITIC ACID	棕榈酸	A	136.5528	HSIAO_LIVER_SPECIFIC_GENES, GO_COFACTOR_METABOLIC_PROCESS, MMP9_subnet, AKT1_subnet, FOS_subnet
L-THREONINE	苏氨酸	A	135.4543	CCND1_subnet, GO_IMMUNE_RESPONSE_REGULATING_CELL_SURFACE_RECEPTOR_SIGNALING_PATHWAY, GMPS_subnet, TOP2B_subnet, TOP2A_subnet
ISOMENTHONE	异薄荷酮	A	134.8237	OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet, OR4S2_subnet, OR51B4_subnet
MENTHONE	薄荷酮	A	134.8237	OR52W1_subnet, OR10S1_subnet, OR2AT4_subnet, OR4S2_subnet, OR51B4_subnet
2-BUTANONE	2-丁酮	A	131.5233	PRKCD_subnet, MDK_subnet, MOOTHA_MITOCHONDRIA, PIK3R3_subnet, MMP14_subnet
BIBENZENE	联二苯	A	130.2413	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, GO_HUMORAL_IMMUNE_RESPONSE, REACTOME_COMPLEMENT_CASCADE
2-ACETYL ANILINE	2-乙酰基苯胺	A	128.2499	ERBB3_subnet, NFATC2_subnet, YES1_subnet, LCK_subnet, BCL6_subnet
ACETIC ACID	醋酸	A	127.8776	GO_DRUG_METABOLIC_PROCESS, FOS_subnet, AKT1_subnet, GNAL_subnet, GNGT1_subnet
L-LEUCINE	亮氨酸	A	127.2245	CCND1_subnet, GMPS_subnet, TOP2B_subnet,

				GO_COFACTOR_METABOLIC_PROCESS, GO_IMMUNE_RESPONSE_REGULATING_CELL_SURFACE_RECEPTOR_SIGNALING_PATHWAY
2,3-DIMETHYLPYRIDINE	2,3-二甲基吡啶	A	124.2705	GO_COFACTOR_METABOLIC_PROCESS, TOP2B_subnet, TOP2A_subnet, MOOTHA_MITOCHONDRIA, BMS1_subnet
L-HISTIDINE	组氨酸	A	122.2688	CCND1_subnet, GO_IMMUNE_RESPONSE_REGULATING_CELL_SURFACE_RECEPTOR_SIGNALING_PATHWAY, HSP90AB1_subnet, GO_ENDOPEPTIDASE_ACTIVITY, RPL5_subnet
CARBOLIC ACID	石碳酸	A	121.6308	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, GO_HUMORAL_IMMUNE_RESPONSE, REACTOME_COMPLEMENT_CASCADE
PHENOL	苯酚	A	121.6308	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, GO_HUMORAL_IMMUNE_RESPONSE, REACTOME_COMPLEMENT_CASCADE
NONANOIC ACID	壬酸	A	121.5204	EGR1_subnet, NFKB1_subnet, GO_REGULATION_OF_VASCULATURE_DEVELOPMENT, MMP9_subnet, AKT1_subnet
CINNAMIC ACID	肉桂酸	A	121.2399	GO_SERINE_HYDROLASE_ACTIVITY, GO_ENDOPEPTIDASE_ACTIVITY, SNAI1_subnet, SOX2_subnet, HSIAO_LIVER_SPECIFIC_GENES
1-AMINO-2-PHENYLETHANE	1-氨基-2-苯基乙烷	A	115.0741	GNAL_subnet, CCND1_subnet, HSP90AB1_subnet, GNGT1_subnet, GO_IMMUNE_RESPONSE_REGULATING_CELL_SURFACE_RECEPTOR_SIGNALING_PATHWAY
ALLYL ISOSULFOCYANATE	异硫氰酸烯丙酯	A	114.3393	ARRB2_subnet, GNGT1_subnet, GRK3_subnet, GNAL_subnet, GO_EXTERNAL_SIDE_OF_PLASMA_MEMBRANE
LOPINAVIR	洛匹那韦	D	113.6459	GSE3920_UNTREATED_VS_IFNB_TREATED_ENDOTHELIAL_CELL_DN, GTPBP4_subnet, NFATC2_subnet, EGR1_subnet, LCK_subnet
PHYTOL	植醇	A	112.6343	ESR2_subnet, PTEN_subnet, WWOX_subnet,

				TGM2_subnet, KDR_subnet
2-BORNANONE	2-炔酮	A	109.0706	GNGT1_subnet, GRK3_subnet, ARRB2_subnet, GNAL_subnet, GO_EXTERNAL_SIDE_OF_PLASMA_MEMBRANE
CAMPHOR	樟脑	A	109.0706	GNGT1_subnet, GRK3_subnet, ARRB2_subnet, GNAL_subnet, GO_EXTERNAL_SIDE_OF_PLASMA_MEMBRANE
D-CAMPHOR	D-樟脑	A	109.0706	GNGT1_subnet, GRK3_subnet, ARRB2_subnet, GNAL_subnet, GO_EXTERNAL_SIDE_OF_PLASMA_MEMBRANE
CYCLOPENTANONE	环戊酮	A	107.9401	MMP9_subnet, EGR1_subnet, MYC_subnet, SRC_subnet, HSP90AB1_subnet
2-METHYL PROPANOIC ACID	2-甲基丙酸	A	101.8336	GO_ENDOPEPTIDASE_ACTIVITY, GO_SERINE_HYDROLASE_ACTIVITY, KEGG_COMPLEMENT_AND_COAGULATION_CASCADES, GO_HUMORAL_IMMUNE_RESPONSE, REACTOME_COMPLEMENT_CASCADE
DIMETHYL RESORCINOL	二甲基间苯二酚	A	101.083	MMP14_subnet, PTPN1_subnet, GO_DRUG_METABOLIC_PROCESS, MMP9_subnet, EGR1_subnet
1-AMINOBUTANE	1-氨基丁烷	A	100.4725	CCND1_subnet, GO_IMMUNE_RESPONSE_REGULATING_CELL_SURFACE_RECEPTOR_SIGNALING_PATHWAY, GO_ENDOPEPTIDASE_ACTIVITY, PRKN_subnet, GMPS_subnet
3-HYDROXY-2-BUTANONE	3-羟基-2-丁酮	A	99.77409	SOX2_subnet, NCOR1_subnet, JUN_subnet, PML_subnet, NFATC1_subnet
ACETOIN	乙醛	A	99.77409	SOX2_subnet, NCOR1_subnet, JUN_subnet, PML_subnet, NFATC1_subnet
ACETYL METHYL CARBINOL	乙酰甲基甲醇	A	99.77409	SOX2_subnet, NCOR1_subnet, JUN_subnet, PML_subnet, NFATC1_subnet
BUTAN-1-OL	丁-1-醇	A	99.08728	LCK_subnet, CTNNB1_subnet, EGFR_subnet, MAPK3_subnet, SRC_subnet

注：“类型"栏标注"D"表示该化合物为初始输入药物，"A"表示芳香化合物。